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Heats of Combustion and Related Properties of Pure Substances

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Abstract

In this work, we compiled and evaluated various properties pertaining to the heats of combustion of about 420 compounds of physical, chemical, and engineering interest. This includes normal boiling points, melting points, latent heats (enthalpies) of vaporization, heats (enthalpies) of fusion, heats (enthalpies) of formation and combustion, and heat capacities (specific heats).

Keywords

Boiling points; combustion; enthalpies; heat capacities; heats of combustion; heats of formation; heats of vaporization; melting points.

Contents

1. Introduction

In this work, we compiled and evaluated various properties pertaining to the heats of combustion of about 400 compounds of physical, chemical, and engineering interest. The information provided here are for hydrocarbons, oxidized hydrocarbons, nitrogen-substituted hydrocarbons, sulfur-substituted hydrocarbons, and halogenated hydrocarbons. The data provided here includes normal boiling points, melting points, latent heats (enthalpies) of vaporization, heats (enthalpies) of fusion, heats (enthalpies) of formation and combustion, and heat capacities (specific heats).

In this Introduction, we first provide an index into the recommended values in Section 2 (Melting and Boiling Points), Section 3 (Heats of Transition), Section 4 (Heats of Combustion, Formation, and Transition), and Section 5 (Heat Capacities). Next in Table 1.1, an alphabetical list of all the compound names (and alternate names) along with the preferred names. For the most part, we used IUPAC standard nomenclature for chemical names, but in some cases used common names (*e.g.*, isobutane vs. 2-methyl propane or acetylene vs. ethyne). We then provide in Table 1.2, information about the compound: the compound name, Chemical Abstracts Registry Number (CASNO), Molecular Formula, and Molecular Weight (MW). In Table 1.3, we provide a list of the compounds along with the chemical classes for each.

In each of the sections, we provide the data for the compounds ordered first by primary/secondary compound class (*e.g.*, Hydrocarbons/Alkanes, Alkenes, etc. or Oxidized Hydrocarbons/Alcohols, Ethers, etc.) and then ordered by molecular formula. The data were taken from many sources in the literature and also from NIST REFPROP [2018LEM], NIST TRC TDE,[2019DIK] and the NIST Chemistry WebBook[2021LIN]. At the end of each section, there is a list of the original source references. We provide uncertainties from the original sources as reported (where available). Our recommended uncertainties are expanded uncertainties U (2σ, 95 % confidence level). The recommended values provided here were selected from reliable original sources (they are not weighted averages) and then an uncertainty was assigned either from the original source, from the range of values, or from our estimate. This is an extensive compilation, however, for some of the compounds and quantities, it is not comprehensive, but there is an adequate selection of values for all compounds from the literature.

Table 1-1. List of Compound Names

Name	Preferred Name
(1-methylethyl)benzene	isopropylbenzene
(1-methylpropyl)benzene	*sec*-butylbenzene
1,1'-bicyclohexyl	1,1'-bicyclohexyl
1,1-dichloroethene	1,1-dichloroethene
1,1-dichloroethylene	1,1-dichloroethene
1,1-difluoroethene	1,1-difluoroethene
1,1-difluoroethylene	1,1-difluoroethene
1,1-dimethyl-1-propanethiol	1,1-dimethyl-1-propanethiol
1,2,3,4-tetrahydronaphthalene	tetralin
1,2-butadiene	1,2-butadiene
1,2-dichloroethene, (*E*)-	1,2-dichloroethene, (*E*)-
1,2-dichloroethene, (*Z*)-	1,2-dichloroethene, (*Z*)-
1,2-dichloroethylene, (*E*)-	1,2-dichloroethene, (*E*)-
1,2-dichloroethylene, (*Z*)-	1,2-dichloroethene, (*Z*)-
1,2-difluoroethene, (*E*)-	1,2-difluoroethene, (*E*)-
1,2-difluoroethene, (*Z*)-	1,2-difluoroethene, (*Z*)-
1,2-difluoroethylene, (*E*)-	1,2-difluoroethene, (*E*)-
1,2-difluoroethylene, (*Z*)-	1,2-difluoroethene, (*Z*)-
1,2-dimethylbenzene	1,2-dimethylbenzene
1,2-ethanediol	1,2-ethanediol
1,2-pentadiene	1,2-pentadiene
1,3,5,7-tetraazaadamantane	methenamine
1,3,5-triazine-2,4,6-triamine	1,3,5-triazine-2,4,6-triamine
1,3-dimethylbenzene	1,3-dimethylbenzene
1,4-dimethylbenzene	1,4-dimethylbenzene
1-methyl-4-isopropylbenzene	*p*-isopropyltoluene
1-oxacyclopent-4-ene-2,5-dione	2,5-furandione
1-propanol	1-propanol
1-propenal	1-propenal
1-propylamine	1-propylamine
2,2-dimethylbutane	neohexane
2,2-dimethylhexane	neooctane
2,2-dimethylpentane	2,2-dimethylpentane
2,2-dimethylpropane	2,2-dimethylpropane
2,2-dimethylpropanethiol	neopentanethiol
2,5-furandione	2,5-furandione
2-bornanone	D-camphor
2-isopropyltoluene	2-isopropyltoluene
2-methyl-1,3-butadiene	2-methyl-1,3-butadiene
2-methyl-1-butanol	2-methyl-1-butanol
2-methyl-1-propanol	isobutanol
2-methyl-2-butanethiol	1,1-dimethyl-1-propanethiol
2-methyl-2-butanol	2-methyl-2-butanol
2-methyl-2-butene	isopentene
2-methyl-2-pentanethiol	tert-pentanethiol
2-methylbutane	isopentane
2-methylhexane	2-methylhexane
2-methyloctane	2-methyloctane
2-methylpentane	isohexane
2-methylpentane	2-methylpentane
2-methylpropan-2-ol	*tert*-butanol
2-methylpropane	isobutane
2-methylpropene	isobutene
2-methylpropylene	isobutene
2-propanol	isopropanol
2-propenal	2-propenal
3-isopropyltoluene	3-isopropyltoluene
3-methyl-1-butanethiol	isopentanethiol
3-methyl-1-butanol	isopentanol
3-methylphenol	3-methylphenol
4-isopropyltoluene	4-isopropyltoluene
acetaldehyde	acetaldehyde
acetone	acetone
acetonitrile	ethane nitrile
acetylene	acetylene
acrolein	2-propenal
allene	allene

aminobenzene	aniline
aniline	aniline
benzocyclohexane	benzocyclohexane
benzocyclopentane	benzocyclopentane
bicyclohexane	1,1'-bicyclohexyl
bromoethene	bromoethene
bromoethylene	bromoethene
bromomethane	bromomethane
butadiyne	butadiyne
butanenitrile	butanenitrile
butanoic acid	butanoic acid
butanone	butanone
butenyne	butenyne
butylamine	*n*-butylamine
carbon tetrachloride	tetrachloromethane
carbonyl dichloride	phosgene
carbonyl fluoride	carbonyl fluoride
chloroethylene	chloroethene
chloroacetylene	chloroacetylene
chloroethane	chloroethane
chloroethene	chloroethene
chloroethyne	chloroacetylene
chloroform	trichloromethane
chloromethane	chloromethane
chlorotrifluoroethene	chlorotrifluoroethene
chlorotrifluoroethylene	chlorotrifluoroethene
cis-decahydronaphthalene	*cis*-decalin
cis-decalin	*cis*-decalin
cumene	isopropylbenzene
cyanoethene	propenenitrile
cyanomethane	ethane nitrile
D-camphor	D-camphor
diacetylene	butadiyne
dichloroacetylene	dichloroacetylene
dichloroethyne	dichloroacetylene
dichloromethane	dichloromethane

diethyl ether	diethyl ether
diisopropyl ether	diisopropyl ether
dimethyl ether	dimethyl ether
dimethyl ketone	acetone
ethanol	ethanol
ethane nitrile	ethane nitrile
ethane	ethane
ethenyl acetate	vinyl acetate
ethenyl bromide	bromoethene
ethenyl ethanoate	vinyl acetate
ethenylbenzene	ethenylbenzene
ethyl 2-propenoate	ethyl 2-propenoate
ethyl acetate	ethyl acetate
ethyl acrylate	ethyl 2-propenoate
ethyl bromide	bromomethane
ethyl chloride	chloroethane
ethyl cyanide	propanenitrile
ethyl ethanoate	ethyl acetate
ethyl ether	diethyl ether
ethyl fluoride	fluoroethane
ethyl formate	ethyl formate
ethyl methanoate	ethyl formate
ethylallene	1,2-pentadiene
ethylene	ethene
ethylene glycol	1,2-ethanediol
ethylene oxide	oxirane
ethyne	acetylene
fluoroethane	fluoroethane
fluoroethene	fluoroethene
fluoroethylene	fluoroethylene
fluoromethane	fluoromethane
formyl fluoride	carbonyl fluoride
furan	furan
glycerin	glycerin
glycerol	glycerin
hexachloroethane	hexachloroethane

hexamethylenetetramine	methenamine
hydrazoic acid	hydrogen azide
hydrogen azide	hydrogen azide
indane	benzocyclopentane
isoamyl alcohol	2-methyl-1-butanol
isobutane	isobutane
isobutanol	isobutanol
Isobutene	isobutene
Isoheptane	2-methylhexane
Isohexane	isohexane
Isononane	2-methyloctane
isooctane	isooctane
isopentane	isopentane
isopentanethiol	isopentanethiol
isopentanol	isopentanol
isopentene	isopentene
isoprene	2-methyl-1,3-butadiene
isopropanol	isopropanol
isopropylbenzene	isopropylbenzene
isopropylether	diisopropyl ether
maleic anhydride	2,5-furandione
m-cresol	3-methylphenol
m-cymene	3-isopropyltoluene
melamine	1,3,5-triazine-2,4,6-triamine
methenamine	methenamine
methyl benzene	toluene
methyl chloride	chloromethane
methyl cyanide	ethane nitrile
methyl ether	dimethyl ether
methyl ethyl ketone	butanone
methyl fluoride	fluoromethane
methyl formate	methyl formate
methyl methacrylate	methyl 2-methylpropenoate
methyl 2-methylpropenoate	methyl 2-methylpropenoate
methyl methonate	methyl formate
methylacetylene	propyne

methylallene	1,2-butadiene
methylene chloride	dichloromethane
methylketene	1-propenal
methyloxacyclopropane	methyloxacyclopropane
methyloxirane	methyloxacyclopropane
m-isopropyltoluene	3-isopropyltoluene
m-xylene	1,3-dimethylbenzene
N,*N*-dimethylaniline	*N*,*N*-dimethylaniline
n-butylamine	*n*-butylamine
neoheptane	2,2-dimethylpentane
neohexane	2,2-dimethylbutane
neohexane	neohexane
neononane	2,2-dimethylheptane
neooctane	neooctane
neopentane	2,2-dimethylpropane
neopentanethiol	neopentanethiol
n-propanol	1-propanol
n-propyl cyanide	butanenitrile
n-propylacetate	*n*-propylacetate
n-propylamine	1-propylamine
o-cymene	2-isopropyltoluene
o-isopropyltoluene	2-isopropyltoluene
oxacyclobutane	oxacyclobutane
oxacyclohexane	oxacyclohexane
oxacyclopentadiene	Furan
oxacyclopropane	oxirane
oxane	oxacyclohexane
oxetane	oxacyclobutane
oxirane	oxirane
o-xylene	1,2-dimethylbenzene
p-cymene	4-isopropyltoluene
perchloroethane	hexachloroethane
phosgene	phosgene
p-isopropyltoluene	4-isopropyltoluene
propadiene	allene
propenenitrile	propenenitrile

propyl acetate	*n*-propylacetate
propyne	propyne
p-xylene	1,4-dimethylbenzene
sec-butylbenzene	*sec*-butylbenzene
styrene	ethenylbenzene
tert-butanol	*tert*-butanol
tert-pentanethiol	*tert*-pentanethiol
tert-pentanol	2-methyl-2-butanol
tetrachloroethene	tetrachloroethene
tetrachloroethylene	tetrachloroethene
tetrachloromethane	tetrachloromethane
tetrafluoroethene	tetrafluoroethene
tetrafluoroethylene	tetrafluoroethene
tetrahydropyran	oxacyclohexane
tetralin	benzocyclohexane
thiacyclopropane	thiacyclopropane

thiirane	thiacyclopropane
toluene	toluene
trans-decahydronaphthalene	*trans*-decalin
trans-decalin	*trans*-decalin
trichloroethene	trichloroethene
trichloroethylene	trichloroethene
trichloromethane	trichloromethane
trifluoroethene	trifluoroethene
trifluoroethylene	trifluoroethene
vinyl acetate	vinyl acetate
vinyl bromide	bromoethene
vinyl chloride	chloroethene
vinyl ethanoate	vinyl acetate
vinylacetylene	butenyne
xylidene	*N*,*N*-dimethylaniline

Table 1-2. Compound Information

Compound	CASNO	Formula	MW
1,1,1,2-tetrachloroethane	106-46-7	$C_2H_2Cl_4$	167.85
1,1,1,2-tetrafluoroethane	811-97-2	$C_2H_2F_4$	102.03
1,1,1-trichloroethane	71-55-6	$C_2H_3Cl_3$	133.40
1,1,1-trifluoroethane	420-46-2	$C_2H_3F_3$	84.04
1,1,2,2-tetrachloroethane	79-34-5	$C_2H_2Cl_4$	167.85
1,1,2,2-tetrafluoroethane	359-35-3	$C_2H_2F_4$	102.03
1,1,2-trichloroethane	79-00-5	$C_2H_3Cl_3$	133.40
1,1,2-trifluoroethane	430-66-0	$C_2H_3F_3$	84.04
1,1'-bicyclohexyl	92-51-3	$C_{12}H_{22}$	166.30
1,1-dichloro-1-fluoroethane	1717-00-6	$C_2H_3Cl_2F$	116.95
1,1-dichloroethane	75-34-3	$C_2H_4Cl_2$	98.96
1,1-dichloroethene	75-35-4	$C_2H_2Cl_2$	96.94
1,1-difluoroethane	75-37-6	$C_2H_4F_2$	66.05
1,1-difluoroethene	75-38-7	$C_2H_2F_2$	64.03
1,1-dimethyl-1-propanethiol	1679-09-0	$C_5H_{12}S$	104.21
1,1-dimethylcyclopentane	1638-26-2	C_7H_{14}	98.19
1,1-dimethylhydrazine	57-14-7	$C_2H_8N_2$	60.10
1,2,3-trimethylbenzene	526-73-8	C_9H_{12}	120.19
1,2,4-trimethylbenzene	95-63-6	C_9H_{12}	120.19
1,2-butadiene	590-19-2	C_4H_6	54.09
1,2-dibromoethane	106-93-4	$C_2H_4Br_2$	187.86
1,2-dichloro-1-fluoroethane	430-57-9	$C_2H_3Cl_2F$	116.95
1,2-dichloro-1-fluoroethene	430-58-0	C_2HCl_2F	114.93
1,2-dichloroethane	107-06-2	$C_2H_4Cl_2$	98.96
1,2-dichloroethene, (*E*)-	156-60-5	$C_2H_2Cl_2$	96.94
1,2-dichloroethene, (*Z*)-	156-59-2	$C_2H_2Cl_2$	96.94
1,2-diethylbenzene	135-01-3	$C_{10}H_{14}$	134.22
1,2-difluoroethane	624-72-6	$C_2H_4F_2$	66.05
1,2-difluoroethene, (*E*)-	1630-78-0	$C_2H_2F_2$	64.03
1,2-difluoroethene, (*Z*)-	1630-77-9	$C_2H_2F_2$	64.03
1,2-dimethylbenzene	95-47-6	C_8H_{10}	106.17
1,2-dimethylcyclohexene	1674-10-8	C_8H_{14}	110.20
1,2-ethanediol	107-21-1	$C_2H_6O_2$	62.07
1,2-pentadiene	591-95-7	C_5H_8	68.12
1,3,5-triazine-2,4,6-triamine	108-78-1	$C_3H_6N_6$	126.12
1,3,5-trimethylbenzene	108-67-8	C_9H_{12}	120.19
1,3,5-trioxane	110-88-3	$C_3H_6O_3$	90.08
1,3-butadiene	106-99-0	C_4H_6	54.09
1,3-cyclohexadiene	592-57-4	C_6H_8	80.13
1,3-cyclopentadiene	542-92-7	C_5H_6	66.10
1,3-diethylbenzene	141-93-5	$C_{10}H_{14}$	134.22
1,3-diethylcyclohexane	1678-99-5	$C_{10}H_{20}$	140.27
1,3-dimethylbenzene	108-38-3	C_8H_{10}	106.17
1,3-dioxane	505-22-6	$C_4H_8O_2$	88.11
1,3-pentadiene	504-60-9	C_5H_8	68.12
1,4-cyclohexadiene	628-41-1	C_6H_8	80.13
1,4-diethylbenzene	105-05-5	$C_{10}H_{14}$	134.22
1,4-dimethylbenzene	106-42-3	C_8H_{10}	106.17
1,4-dioxane	123-91-1	$C_4H_8O_2$	88.11
1,4-pentadiene	591-93-5	C_5H_8	68.12
1,5-cyclooctadiene	111-78-4	C_8H_{12}	108.18
1-butanethiol	109-79-5	$C_4H_{10}S$	90.19
1-butanol	71-36-3	$C_4H_{10}O$	74.12
1-butene	106-98-9	C_4H_8	56.11
1-butyne	107-00-6	C_4H_6	54.09
1-chloro-1,1-difluoroethane	75-68-3	$C_2H_3ClF_2$	100.50
1-chloro-1-fluoroethane	1615-75-4	C_2H_4ClF	82.50
1-chloro-2,2-difluoroethane	338-65-8	$C_2H_3ClF_2$	100.50
1-decene	872-05-9	$C_{10}H_{20}$	140.27
1-ethylcyclohexene	1453-24-3	C_8H_{14}	110.20
1-ethylcyclopentene	2146-38-5	C_7H_{12}	96.17
1-heptanethiol	1639-09-4	$C_7H_{16}S$	132.27
1-heptene	592-76-7	C_7H_{14}	98.19
1-heptyne	628-71-7	C_7H_{12}	96.17
1-hexanethiol	111-31-9	$C_6H_{14}S$	118.24
1-hexene	592-41-6	C_6H_{12}	84.16
1-hexyne	693-02-7	C_6H_{10}	82.14
1-isobutanethiol	513-44-0	$C_4H_{10}S$	90.19
1-methyl-2-ethylbenzene	611-14-3	C_9H_{12}	120.19

1-methyl-3-ethylbenzene	620-14-4	C_9H_{12}	120.19
1-methyl-4-ethylbenzene	622-96-8	C_9H_{12}	120.19
1-methylcyclohexene	591-49-1	C_7H_{12}	96.17
1-methylnaphthalene	90-12-0	$C_{11}H_{10}$	142.20
1-methylpyrrole	96-54-8	C_5H_7N	81.12
1-nonene	124-11-8	C_9H_{18}	126.24
1-octene	111-66-0	C_8H_{16}	112.21
1-octyne	629-05-0	$C_{11}H_{14}$	146.23
1-pentanethiol	110-66-7	$C_5H_{12}S$	104.21
1-pentanol	71-41-0	$C_5H_{12}O$	88.15
1-penten-3-yne	646-05-9	C_5H_6	66.10
1-pentene	109-67-1	C_5H_{10}	70.13
1-pentyne	627-19-0	C_5H_8	68.12
1-propanethiol	107-03-9	C_3H_8S	76.16
1-propanol	71-23-8	C_3H_8O	60.10
1-propenal	6004-44-0	C_3H_4O	56.06
1-propylamine	107-10-8	C_3H_9N	59.11
2,2,3-trimethylbutane	464-06-2	C_7H_{16}	100.20
2,2,4-trimethylpentane	540-84-1	C_8H_{18}	114.23
2,2-dimethylhexane	590-73-8	C_8H_{18}	114.23
2,3-dimethylbutane	79-29-8	C_6H_{14}	86.18
2,3-dimethylpentane	565-59-3	C_7H_{16}	100.20
2,4-diisocyanatotoluene	584-84-9	$C_9H_6N_2O_2$	174.16
2,4-dimethylpentane	108-08-7	C_7H_{16}	100.20
2,5-furandione	108-31-6	$C_4H_2O_3$	98.06
2-butanethiol	513-53-1	$C_4H_{10}S$	90.19
2-butanol	78-92-2	$C_4H_{10}O$	74.12
2-butene, (*E*)-	624-64-6	C_4H_8	56.11
2-butene, (*Z*)-	590-18-1	C_4H_8	56.11
2-butyne	503-17-3	C_4H_6	54.09
2-chloro-1,1,1-trifluoroethane	75-88-7	$C_2H_2ClF_3$	118.49
2-hexyne	764-35-2	C_6H_{10}	82.14
2-isopropyltoluene	527-84-4	$C_{10}H_{14}$	134.22
2-methoxyethanol	109-86-4	$C_3H_8O_2$	76.09
2-methyl-1,3-butadiene	78-79-5	C_5H_8	68.12
2-methyl-1-butanol	137-32-6	$C_5H_{12}O$	88.15
2-methyl-1-butene	563-46-2	C_5H_{10}	70.13

2-methyl-2-butanol	75-85-4	$C_5H_{12}O$	88.15
2-methyl-2-butene	513-35-9	C_5H_{10}	70.13
2-methylcyclohexanone	583-60-8	$C_7H_{12}O$	112.17
2-methylfuran	534-22-5	C_5H_6O	82.10
2-methylheptane	592-27-8	C_8H_{18}	114.23
2-methylnaphthalene	91-57-6	$C_{11}H_{10}$	142.20
2-methylphenol	95-48-7	C_7H_8O	108.14
2-methylpyridine	109-06-8	C_6H_7N	93.13
2-pentanol	6032-29-7	$C_5H_{12}O$	88.15
2-pentanone	107-87-9	$C_5H_{10}O$	86.13
2-pentene, (*E*)-	646-04-8	C_5H_{10}	70.13
2-pentene, (*Z*)-	627-20-3	C_5H_{10}	70.13
2-pentyne	627-21-4	C_5H_8	68.12
2-propenal	107-02-8	C_3H_4O	56.06
3,3-dimethylpentane	562-49-2	C_7H_{16}	100.20
3-ethylcyclopentene	694-35-9	C_7H_{12}	96.17
3-hexyne	928-49-4	C_6H_{10}	82.14
3-isopropyltoluene	535-77-3	$C_{10}H_{14}$	134.22
3-methyl-1-butene	563-45-1	C_5H_{10}	70.13
3-methyl-2-butanol	598-75-4	$C_5H_{12}O$	88.15
3-methylcyclohexanone	591-24-2	$C_7H_{12}O$	112.17
3-methylcyclopentene	1120-62-3	C_6H_{10}	82.14
3-methylhexane	589-34-4	C_7H_{16}	100.20
3-methylpentane	96-14-0	C_6H_{14}	86.18
3-methylphenol	108-39-4	C_7H_8O	108.14
3-pentanol	584-02-1	$C_5H_{12}O$	88.15
3-pentanone	96-22-0	$C_5H_{10}O$	86.13
3-penten-1-yne	2206-23-7	C_5H_6	66.10
4-isopropyltoluene	99-87-6	$C_{10}H_{14}$	134.22
4-methylcyclohexanone	589-92-4	$C_7H_{12}O$	112.17
4-methylphenol	106-44-5	C_7H_8O	108.14
acenaphthene	83-32-9	$C_{12}H_{10}$	154.21
acenaphthylene	208-96-8	$C_{12}H_8$	152.19
acetaldehyde	75-07-0	C_2H_4O	44.05
acetic acid	64-19-7	$C_2H_4O_2$	60.05
acetic anhydride	108-24-7	$C_4H_6O_3$	102.09
acetone	67-64-1	C_3H_6O	58.08

acetylene	74-86-2	C_2H_2	26.04
allene	463-49-0	C_3H_4	40.06
alpha-D-glucose	492-62-6	$C_6H_{12}O_6$	180.16
ammonia	7664-41-7	H_3N	17.03
ammonium perchlorate	7790-98-9	ClH_4NO_4	117.49
aniline	62-53-3	C_6H_7N	93.13
anthracene	120-12-7	$C_{14}H_{10}$	178.23
azacyclobutane	503-29-7	C_3H_7N	57.09
azacyclopentane	123-75-1	C_4H_9N	71.12
azacyclopropane	151-56-4	C_2H_5N	43.07
benzaldehyde	100-52-7	C_7H_6O	106.12
benzene	71-43-2	C_6H_6	78.11
benzenethiol	108-98-5	C_6H_6S	110.18
benzoic acid	65-85-0	$C_7H_6O_2$	122.12
benzyl alcohol	100-51-6	C_7H_8O	108.14
biphenylene	259-79-0	$C_{12}H_8$	152.19
bromochlorodifluoromethane	353-59-3	$CBrClF_2$	165.36
bromochlorofluoromethane	593-98-6	$CHBrClF$	147.37
bromochloromethane	74-97-5	CH_2BrCl	129.38
bromodichlorofluoromethane	353-58-2	$CBrCl_2F$	181.82
bromodichloromethane	75-27-4	$CHBrCl_2$	163.83
bromodifluoromethane	1511-62-2	$CHBrF_2$	130.92
bromoethane	74-96-4	C_2H_5Br	108.97
bromoethene	593-60-2	C_2H_3Br	106.95
bromofluoromethane	373-52-4	CH_2BrF	112.93
bromomethane	74-83-9	CH_3Br	94.94
bromotrichloromethane	75-62-7	$CBrCl_3$	198.27
bromotrifluoromethane	75-63-8	$CBrF_3$	148.91
butadiyne	460-12-8	C_4H_2	50.06
butanal	123-72-8	C_4H_8O	72.11
butanenitrile	109-74-0	C_4H_7N	69.11
butanoic acid	107-92-6	$C_4H_8O_2$	88.11
butanoic anhydride	106-31-0	$C_8H_{14}O_3$	158.19
butanone	78-93-3	C_4H_8O	72.11
butenyne	689-97-4	C_4H_4	52.07
carbon	7440-44-0	C	12.01
carbon dioxide	124-38-9	CO_2	44.01
carbon disulfide	75-15-0	CS_2	76.14
carbon monoxide	630-08-0	CO	28.01
carbonyl difluoride	353-50-4	CF_2O	66.01
carbonyl fluoride	1493-02-3	CHFO	48.02
chlorobenzene	108-90-7	C_6H_5Cl	112.56
chlorodifluoromethane	75-45-6	$CHClF_2$	86.47
chloroethane	75-00-3	C_2H_5Cl	64.51
chloroethene	75-01-4	C_2H_3Cl	62.50
chloroacetylene	593-63-5	C_2HCl	60.48
chlorofluoromethane	593-70-4	CH_2ClF	68.48
chloromethane	74-87-3	CH_3Cl	50.49
chlorotrifluoroethene	79-38-9	C_2ClF_3	116.47
chlorotrifluoromethane	75-72-9	$CClF_3$	104.46
cis-decalin	493-01-6	$C_{10}H_{18}$	138.25
coronene	191-07-1	$C_{24}H_{12}$	300.35
cyanogen	460-19-5	C_2N_2	52.03
cyclobutadiene	1120-53-2	C_4H_4	52.07
cyclobutane	287-23-0	C_4H_8	56.11
cyclobutanone	1191-95-3	C_4H_6O	70.09
cyclobutene	822-35-5	C_4H_6	54.09
cycloheptane	291-64-5	C_7H_{14}	98.19
cycloheptene	628-92-2	C_7H_{12}	96.17
cyclohexane	110-82-7	C_6H_{12}	84.16
cyclohexanone	108-94-1	$C_6H_{10}O$	98.14
cyclohexene	110-83-8	C_6H_{10}	82.14
cyclohexylamine	108-91-8	$C_6H_{13}N$	99.17
cyclopentane	287-92-3	C_5H_{10}	70.13
cyclopentanone	120-92-3	C_5H_8O	84.12
cyclopentene	142-29-0	C_5H_8	68.12
cyclopropane	75-19-4	C_3H_6	42.08
cyclopropanone	5009-27-8	C_3H_4O	56.06
cyclopropene	2781-85-3	C_3H_4	40.06
D-camphor	76-22-2	$C_{10}H_{16}O$	152.23
diborane	19287-45-7	B_2H_6	16.86
dibromochlorofluoromethane	353-55-9	CBr_2ClF	226.27
dibromochloromethane	124-48-1	$CHBr_2Cl$	208.28
dibromochloromethane	124-48-1	$CHBr_2Cl$	208.28

dibromodichloromethane	594-18-3	CBr_2Cl_2	242.72
dibromodifluoromethane	75-61-6	CBr_2F_2	209.82
dibromofluoromethane	1868-53-7	$CHBr_2F$	191.83
dibromomethane	74-95-3	CH_2Br_2	173.83
dichlorodifluoromethane	75-71-8	CCl_2F_2	120.91
dichloroacetylene	7572-29-4	C_2Cl_2	94.93
dichlorofluoromethane	75-43-4	$CHCl_2F$	102.92
dichloromethane	75-09-2	CH_2Cl_2	84.93
diethyl ether	60-29-7	$C_4H_{10}O$	74.12
diethyl sulfide	352-93-2	$C_4H_{10}S$	90.19
diethylamine	109-89-7	$C_4H_{11}N$	73.14
difluorochloromethane	75-45-6	$CHClF_2$	86.47
difluoroethyne	689-99-6	C_2F_2	62.02
difluoromethane	75-10-5	CH_2F_2	52.02
diisopropyl ether	108-20-3	$C_6H_{14}O$	102.17
dimethyl disulfide	624-92-0	$C_2H_6S_2$	94.20
dimethyl ether	115-10-6	C_2H_6O	46.07
dimethyl sulfide	75-18-3	C_2H_6S	62.13
dimethyl sulfoxide	67-68-5	C_2H_6OS	78.13
dimethylamine	124-40-3	C_2H_7N	45.08
di-*n*-butyl sulfide	544-40-1	$C_8H_{18}S$	146.29
di-*n*-propyl ether	111-43-3	$C_6H_{14}O$	102.17
di-*n*-propyl sulfide	111-47-7	$C_6H_{14}S$	118.24
ethane	74-84-0	C_2H_6	30.07
ethanenitrile	75-05-8	C_2H_3N	41.05
ethanethiol	75-08-1	C_2H_6S	62.13
ethanol	64-17-5	C_2H_6O	46.07
ethene	74-85-1	C_2H_4	28.05
ethenylbenzene	100-42-5	C_8H_8	104.15
ethyl acetate	141-78-6	$C_4H_8O_2$	88.11
ethyl propenoate	140-88-5	$C_5H_8O_2$	100.12
ethyl formate	109-94-4	$C_4H_6O_2$	86.09
ethyl isopropyl sulfide	5145-99-3	$C_5H_{12}S$	104.21
ethyl methyl ether	540-67-0	C_3H_8O	60.10
ethyl methyl sulfide	624-89-5	C_3H_8S	76.16
ethyl propyl sulfide	4110-50-3	$C_5H_{12}S$	104.21
ethylamine	75-04-7	C_2H_7N	45.08

ethylbenzene	100-41-4	C_8H_{10}	106.17
ethylcyclohexane	1678-91-7	C_8H_{16}	112.21
ethylcyclopentane	1640-89-7	C_7H_{14}	98.19
fluoranthene	206-44-0	$C_{16}H_{10}$	202.25
fluorene	86-73-7	$C_{13}H_{10}$	166.22
fluoroethane	353-36-6	C_2H_5F	48.06
fluoroethene	75-02-5	$C_2H_3F_3$	84.04
fluoroethyne	2713-09-9	C_2HF	44.03
fluoromethane	593-53-3	CH_3F	34.03
formaldehyde	50-00-0	CH_2O	30.03
formic acid	64-18-6	CH_2O_2	46.03
furan	110-00-9	C_4H_4O	68.07
glycerin	56-81-5	$C_3H_8O_3$	92.09
graphite	7782-42-5	C	12.01
hexachloroethane	67-72-1	C_2Cl_6	236.74
hexafluoroethane	76-16-4	C_2F_6	138.01
hexamethyldisiloxane	107-46-0	$C_6H_{18}OSi_2$	162.38
hexanenitrile	628-73-9	$C_6H_{11}N$	97.16
hydrazine	302-01-2	H_4N_2	32.05
hydrogen	1333-74-0	H_2	2.02
hydrogen azide	7782-79-8	HN_3	43.03
hydrogen cyanide	74-90-8	CHN	27.03
hydrogen peroxide	7722-84-1	H_2O_2	34.01
hydrogen sulfide	7783-06-4	H_2S	34.08
indane	496-11-7	C_9H_{10}	118.18
indene	95-13-6	C_9H_8	116.16
iodomethane	74-88-4	CH_3I	141.94
isobutanal	78-84-2	C_4H_8O	72.11
isobutane	75-28-5	C_4H_{10}	58.12
isobutanol	78-83-1	$C_4H_{10}O$	74.12
isobutene	115-11-7	C_4H_8	56.11
isobutyl ethyl ether	628-81-9	$C_6H_{14}O$	102.17
isobutylamine	78-81-9	$C_4H_{11}N$	73.14
Isobutylbenzene	538-93-2	$C_{10}H_{14}$	134.22
isobutylcyclohexane	1678-98-4	$C_{10}H_{20}$	140.27
isoheptane	591-76-4	C_7H_{16}	100.20
isohexane	107-83-5	C_6H_{14}	86.18

isononane	3221-61-2	C_9H_{20}	128.26
isopentane	78-78-4	C_5H_{12}	72.15
isopentanethiol	541-31-1	$C_5H_{12}S$	104.21
isopentanol	123-51-3	$C_5H_{12}O$	88.15
isopropanethiol	75-33-2	C_3H_8S	76.16
isopropanol	67-63-0	C_3H_8O	60.10
isopropyl methyl ether	598-53-8	$C_4H_{10}O$	74.12
isopropyl methyl sulfide	1551-21-9	$C_4H_{10}S$	90.19
isopropylamine	75-31-0	C_3H_9N	59.11
isopropylbenzene	98-82-8	C_9H_{12}	120.19
isopropylcyclohexane	696-29-7	C_9H_{18}	126.24
isopropylcyclopentane	3875-51-2	C_8H_{16}	112.21
methane	74-82-8	CH_4	16.04
methanethiol	74-93-1	CH_4S	48.11
methanol	67-56-1	CH_4O	32.04
methenamine	100-97-0	$C_6H_{12}N_4$	140.19
methyl acetate	79-20-9	$C_3H_6O_2$	74.08
methyl butanoate	623-42-7	$C_5H_{10}O_2$	102.13
methyl formate	107-31-3	$C_4H_6O_2$	86.09
methyl isopropyl sulfide	1551-21-9	$C_4H_{10}S$	90.19
methyl 2-methylpropenoate	80-62-6	$C_5H_8O_2$	100.12
methyl nitrate	598-58-3	CH_3NO_3	77.04
methyl propanoate	554-12-1	$C_4H_8O_2$	88.11
methyl propyl sulfide	3877-15-4	$C_4H_{10}S$	90.19
methylamine	74-89-5	CH_5N	31.06
methylcyclobutane	598-61-8	C_5H_{10}	70.13
methylcyclohexane	108-87-2	C_7H_{14}	98.19
methylcyclopentane	96-37-7	C_6H_{12}	84.16
methylenecyclobutane	1120-56-5	C_5H_8	68.12
methylenecyclohexane	1192-37-6	C_7H_{12}	96.17
methylethylamine	624-78-2	C_3H_9N	59.11
methyloxacyclopropane	75-56-9	C_3H_6O	58.08
N,*N*-dimethylaniline	121-69-7	$C_8H_{11}N$	121.18
naphthacene	92-24-0	$C_{18}H_{12}$	228.29
naphthalene	91-20-3	$C_{10}H_8$	128.17
n-butane	106-97-8	C_4H_{10}	58.12
n-butanoic acid	107-92-6	C_4H_8O	88.11
n-butyl methyl ether	628-28-4	$C_5H_{12}O$	88.15
n-butylamine	109-73-9	$C_4H_{11}N$	73.14
n-butylbenzene	104-51-8	$C_{10}H_{14}$	134.22
n-decane	124-18-5	$C_{10}H_{22}$	142.28
n-dodecane	112-40-3	$C_{12}H_{26}$	170.33
neoheptane	590-35-2	C_7H_{16}	100.20
neohexane	75-83-2	C_6H_{14}	86.18
neononane	1071-26-7	C_9H_{20}	128.26
neopentane	463-82-1	C_5H_{12}	72.15
neopentanethiol	1679-08-9	$C_5H_{12}S$	104.21
n-heptane	142-82-5	C_7H_{16}	100.20
n-hexadecane	544-76-3	$C_{16}H_{34}$	226.44
n-hexane	110-54-3	C_6H_{14}	86.18
n-hexanoic acid	142-62-	$C_6H_{12}O_2$	116.16
nitrobenzene	98-95-3	$C_6H_5NO_2$	123.11
nitrogen	7727-37-9	N_2	28.01
nitroglycerin	55-63-0	$C_3H_5N_3O_9$	227.09
nitromethane	75-52-5	CH_3NO_2	61.04
nitrous oxide	10024-97-2	N_2O	44.01
n-nonane	111-84-2	C_9H_{20}	128.26
n-octane	111-65-9	C_8H_{18}	114.23
n-pentane	109-66-0	C_5H_{12}	72.15
n-pentanoic acid	109-52-4	$C_5H_{10}O$	86.13
n-propyl methyl ether	557-17-5	$C_4H_{10}O$	74.12
n-propylacetate	109-60-4	$C_5H_{10}O_2$	102.13
n-propylbenzene	103-65-1	C_9H_{12}	120.19
n-propylcyclopentane	2040-96-2	C_8H_{16}	112.21
n-undecane	1120-21-4	$C_{11}H_{24}$	156.31
octamethylcyclotetrasiloxane	556-67-2	$C_8H_{24}O_4Si_4$	296.62
oxacyclobutane	503-30-0	C_3H_6O	58.08
oxacyclohexane	142-68-7	$C_5H_{10}O$	86.13
oxacyclopentane	109-99-9	C_4H_8O	72.11
oxirane	75-21-8	C_2H_4O	44.05
oxygen	7782-44-7	O_2	32.00
pentachloroethane	76-01-7	C_2HCl_5	202.29
pentachlorophenol	87-86-5	C_6HCl_5O	266.34
pentafluoroethane	354-33-6	C_2HF_5	120.02

pentanenitrile	110-59-8	C_5H_9N	83.13
perylene	198-55-0	$C_{20}H_{12}$	252.31
phenanthrene	85-01-8	$C_{14}H_{10}$	178.23
phenol	108-95-2	C_6H_6O	94.11
phosgene	75-44-5	CCl_2O	98.92
piperidine	110-89-4	$C_5H_{11}N$	85.15
propanal	123-38-6	C_3H_6O	58.08
propane	74-98-6	C_3H_8	44.10
propanenitrile	107-12-0	C_3H_5N	55.08
propanoic acid	79-09-4	$C_3H_6O_2$	74.08
propanoic anhydride	123-62-6	$C_6H_{10}O_3$	130.14
propene	115-07-1	C_3H_6	42.08
propenenitrile	107-13-1	C_3H_3N	53.06
propylcyclohexane	1678-92-8	C_9H_{18}	126.24
propyne	74-99-7	C_3H_4	40.06
pyrene	129-00-0	$C_{16}H_{10}$	202.25
pyrrole	109-97-7	C_4H_5N	67.09
sec-butylbenzene	135-98-8	$C_{10}H_{14}$	134.22
sucrose	57-50-1	$C_{12}H_{22}O_{11}$	342.30
sulfur dioxide	7446-09-5	O_2S	64.06
tert-butanol	75-65-0	$C_4H_{10}O$	74.12
tert-butyl methyl ether	1634-04-4	$C_5H_{12}O$	88.15
tert-butylamine	75-64-9	$C_4H_{11}N$	73.14
tert-butylbenzene	98-06-6	$C_{10}H_{14}$	134.22
tert-butylcyclohexane	3178-22-1	$C_{10}H_{20}$	140.27
tert-pentanethiol	1679-09-0	$C_5H_{12}S$	104.21
tetrabromomethane	558-13-4	CBr_4	331.63
tetrachloroethene	127-18-4	C_2Cl_4	165.83
tetrachloromethane	56-23-5	CCl_4	153.82
tetrafluoroethene	116-14-3	C_2F_4	100.02
tetrafluoromethane	75-73-0	CF_4	88.00
tetralin	119-64-2	$C_{10}H_{12}$	132.20
tetranitromethane	509-14-8	CN_4O_8	196.03
thiacyclobutane	287-27-4	C_3H_6S	74.14
thiacyclohexane	1613-51-0	$C_5H_{10}S$	102.20
thiacyclopentane	110-01-0	C_4H_8S	88.17
thiacyclopropane	420-12-2	C_2H_4S	60.12
thiophene	110-02-1	C_4H_4S	84.14
toluene	108-88-3	C_7H_8	92.14
trans-decalin	493-02-7	$C_{10}H_{18}$	138.25
tribromochloromethane	594-15-0	CBr_3Cl	287.18
tribromofluoromethane	353-54-8	CBr_3F	270.72
tribromomethane	75-25-2	$CHBr_3$	252.73
trichloroethene	79-01-6	C_2HCl_3	131.39
trichlorofluoromethane	75-69-4	CCl_3F	137.37
trichloromethane	67-66-3	$CHCl_3$	119.38
triethanolamine	102-71-6	$C_6H_{15}NO_3$	149.19
triethylamine	121-44-8	$C_6H_{15}N$	101.19
trifluoroethene	359-11-5	C_2HF_3	82.02
trifluoromethane	75-46-7	CHF_3	70.01
trimethylamine	75-50-3	C_3H_9N	59.11
trinitromethane	517-25-9	CHN_3O_6	151.04
trinitrotoluene	118-96-7	$C_7H_5N_3O_6$	227.13
urea	57-13-6	CH_4N_2O	60.06
vinyl acetate	108-05-4	$C_4H_6O_2$	86.09
water	7732-18-5	H_2O	18.02

Table 1-3. Classes of Compounds

Compound	Class
1,1,1,2-tetrachloroethane	Chloroalkanes
1,1,1,2-tetrafluoroethane	Fluoroalkanes
1,1,1-trichloroethane	Chloroalkanes
1,1,1-trifluoroethane	Fluoroalkanes
1,1,2,2-tetrachloroethane	Chloroalkanes
1,1,2,2-tetrafluoroethane	Fluoroalkanes
1,1,2-trichloroethane	Chloroalkanes
1,1,2-trifluoroethane	Fluoroalkanes
1,1'-bicyclohexyl	Bicycloalkanes
1,1-dichloroethane	Chloroalkanes
1,1-dichloroethene	Chloroalkenes
1,1-difluoroethane	Fluoroalkanes
1,1-difluoroethene	Fluoroalkenes
1,1-dimethyl-1-propanethiol	Alkanethiols
1,1-dimethylcyclopentane	Cycloalkanes
1,1-dimethylhydrazine	Cyanogen
1,2,3-trimethylbenzene	Aromatic Hydrocarbons
1,2,4-trimethylbenzene	Aromatic Hydrocarbons
1,2-butadiene	Alkenes
1,2-dichloroethane	Chloroalkanes
1,2-dichloroethene, (*E*)-	Chloroalkenes
1,2-dichloroethene, (Z)-	Chloroalkenes
1,2-diethylbenzene	Aromatic Hydrocarbons
1,2-difluoroethene, (*E*)-	Fluoroalkenes
1,2-difluoroethene, (Z)-	Fluoroalkenes
1,2-dimethylbenzene	Aromatic Hydrocarbons
1,2-ethanediol	Sugars and Ethanediol
1,2-pentadiene	Alkenes
1,3,5-triazine-2,4,6-triamine	Cyanogen
1,3,5-trimethylbenzene	Aromatic Hydrocarbons
1,3,5-trioxane	Dixoanes and Trioxanes
1,3-butadiene	Alkenes
1,3-cyclohexadiene	Cycloalkenes
1,3-cyclopentadiene	Cycloalkenes
1,3-diethylbenzene	Aromatic Hydrocarbons
1,3-diethylcyclohexane	Cycloalkanes
1,3-dimethylbenzene	Aromatic Hydrocarbons
1,3-dioxane	Dixoanes and Trioxanes
1,3-pentadiene	Alkenes
1,4-dimethylbenzene	Aromatic Hydrocarbons
1,4-diethylbenzene	Aromatic Hydrocarbons
1,4-dioxane	Dixoanes and Trioxanes
1,4-pentadiene	Alkenes
1-butanethiol	Alkanethiols
1-butanol	Alkanols
1-butene	Alkenes
1-butyne	Alkynes
1-decene	Alkenes
1-heptanethiol	Alkanethiols
1-heptene	Alkenes
1-hexanethiol	Alkanethiols
1-hexene	Alkenes
1-hexyne	Alkynes
1-isobutanethiol	Alkanethiols
1-methyl-2-ethylbenzene	Aromatic Hydrocarbons
1-methyl-3-ethylbenzene	Aromatic Hydrocarbons
1-methyl-4-ethylbenzene	Aromatic Hydrocarbons
1-methylnaphthalene	Aromatic Hydrocarbons
1-methylpyrrole	Cycloalkylamines
1-nonene	Alkenes
1-octene	Alkenes
1-pentanethiol	Alkanethiols
1-pentanol	Alkanols
1-pentene	Alkenes
1-pentyne	Alkynes
1-propanethiol	Alkanethiols
1-propanol	Alkanols
1-propylamine	Alkylamines
2,2,3-trimethylbutane	Alkanes

2,2-dimethylhexane	Alkanes
2,3-dimethylbutane	Alkanes
2,3-dimethylpentane	Alkanes
2,4-diisocyanatotoluene	Aromatic CHNOx
2,5-furandione	Camphor and Furandione
2-butanethiol	Alkanethiols
2-butanol	Alkanols
2-butene, (*E*)-	Alkenes
2-butene, (Z)-	Alkenes
2-hexyne	Alkynes
2-isopropyltoluene	Aromatic Hydrocarbons
2-methoxyethanol	Sugars and Ethanediol
2-methyl-1-butanol	Alkanols
2-methyl-1-butene	Alkenes
2-methyl-2-butene	Alkenes
2-methylfuran	Oxacycloalkanes
2-methylnaphthalene	Aromatic Hydrocarbons
2-methylphenol	Aromatic Alcohols
2-methylpyridine	Aromatic Amines
2-pentanol	Alkanols
2-pentene, (*E*)-	Alkenes
2-pentene, (Z)-	Alkenes
2-pentyne	Alkynes
2-propenal	Aldehydes
3,3-dimethylpentane	Alkanes
3-hexyne	Alkynes
3-isopropyltoluene	Aromatic Hydrocarbons
3-methyl-1-butene	Alkenes
3-methylhexane	Alkanes
3-methylpentane	Alkanes
3-methylphenol	Aromatic Alcohols
3-pentanone	Ketones
3-penten-1-yne	Alkynes
4-isopropyltoluene	Aromatic Hydrocarbons
4-methylphenol	Aromatic Alcohols
acenaphthene	Polycyclic Aromatic Hydrocarbons
acenaphthylene	Polycyclic Aromatic Hydrocarbons

acetaldehyde	Aldehydes
acetic acid	Carboxylic Acids
acetone	Ketones
acetylene	Alkynes
allene	Alkenes
alpha-D-glucose	Sugars and Ethanediol
ammonia	Nitrogen/Hydrogen
aniline	Aromatic Amines
anthracene	Polycyclic Aromatic Hydrocarbons
azacyclopentane	Cycloalkylamines
benzaldehyde	Aromatic Alcohols
benzene	Aromatic Hydrocarbons
benzenethiol	Sulfur-Substituted Cyclohydrocarbons
benzoic acid	Aromatic Alcohols
benzyl alcohol	Aromatic Alcohols
biphenylene	Polycyclic Aromatic Hydrocarbons
bromochlorodifluoromethane	Bromochlorofluoroalkanes
bromochlorofluoromethane	Bromochlorofluoroalkanes
bromochloromethane	Bromofluoroalkanes
bromodichlorofluoromethane	Bromochlorofluoroalkanes
bromodichloromethane	Bromochloroalkanes
bromodifluoromethane	Bromofluoroalkanes
bromoethane	Bromoalkanes
bromoethene	Bromoalkenes
bromofluoromethane	Bromofluoroalkanes
bromomethane	Bromoalkanes
bromotrichloromethane	Bromochloroalkanes
bromotrifluoromethane	Bromofluoroalkanes
butadiyne	Alkynes
butanal	Aldehydes
butanenitrile	Alkanenitriles
butanone	Ketones
butenyne	Alkynes
carbon dioxide	Carbon Monoxide, Carbon Dioxide
carbon disulfide	Alkyl Sulfides
carbon monoxide	Carbon Monoxide, Carbon Dioxide
carbonyl difluoride	Carbonyl Halides

chlorobenzene	Chlorobenzene
chlorodifluoromethane	Chlorofluoroalkanes
chloroethane	Chloroalkanes
chloroethene	Chloroalkenes
chlorofluoromethane	Chlorofluoroalkanes
chloromethane	Chloroalkanes
chlorotrifluoroethene	Chlorofluoroalkenes
chlorotrifluoromethane	Chlorofluoroalkanes
cis-decalin	Bicycloalkanes
coronene	Polycyclic Aromatic Hydrocarbons
cyanogen	Cyanogen
cyclobutane	Cycloalkanes
cyclobutanone	Cycloalkanones
cyclobutene	Cycloalkenes
cyclohexane	Cycloalkanes
cyclohexanone	Cycloalkanones
cyclohexene	Cycloalkenes
cyclohexylamine	Cycloalkylamines
cyclopentane	Cycloalkanes
cyclopentene	Cycloalkenes
cyclopropane	Cycloalkanes
D-camphor	Camphor and Furandione
diborane	Boron/Hydrogen
dibromochlorofluoromethane	Bromochlorofluoroalkanes
dibromochloromethane	Bromochloroalkanes
dibromodichloromethane	Bromochloroalkanes
dibromodifluoromethane	Bromofluoroalkanes
dibromomethane	Bromoalkanes
dichlorodifluoromethane	Chlorofluoroalkanes
dichlorofluoromethane	Chlorofluoroalkanes
dichloromethane	Chloroalkanes
diethyl ether	Ethers
diethyl sulfide	Alkyl Sulfides
difluoromethane	Fluoroalkanes
diisopropyl ether	Ethers
dimethyl disulfide	Alkyl Sulfides
dimethyl ether	Ethers
dimethyl sulfide	Alkyl Sulfides
dimethyl sulfoxide	Dimethyl Sulfoxide
dimethylamine	Alkylamines
di-*n*-propyl ether	Ethers
ethane	Alkanes
ethanenitrile	Alkanenitriles
ethanethiol	Alkanethiols
ethanol	Alkanols
ethene	Alkenes
ethyl acetate	Esters
ethyl propenoate	Esters
ethyl formate	Esters
ethyl methyl sulfide	Alkyl Sulfides
ethylamine	Alkylamines
ethylbenzene	Aromatic Hydrocarbons
ethylcyclopentane	Cycloalkanes
fluoranthene	Polycyclic Aromatic Hydrocarbons
fluorene	Polycyclic Aromatic Hydrocarbons
fluoroethane	Fluoroalkanes
fluoroethene	Fluoroalkenes
fluoromethane	Fluoroalkanes
formaldehyde	Aldehydes
formic acid	Carboxylic Acids
furan	Oxacycloalkanes
glycerin	Sugars and Ethanediol
hexachloroethane	Chloroalkanes
hexafluoroethane	Fluoroalkanes
hexamethyldisiloxane	Siloxanes
hexanenitrile	Alkanenitriles
hydrogen	Hydrogen/Oxygen
hydrogen cyanide	Hydrogen Cyanide
hydrogen peroxide	Hydrogen/Oxygen
hydrogen sulfide	Nitrogen/Hydrogen
indene	Aromatic Hydrocarbons
isobutanal	Aldehydes
isobutane	Alkanes
isobutanol	Alkanols

isobutene	Alkenes
isobutylcyclohexane	Cycloalkanes
isoheptane	Alkanes
isohexane	Alkanes
isooctane	Alkanes
isopentane	Alkanes
isopentanol	Alkanols
isoprene	Alkenes
isopropanethiol	Alkanethiols
isopropanol	Alkanols
isopropylamine	Alkylamines
isopropylbenzene	Aromatic Hydrocarbons
isopropylcyclohexane	Cycloalkanes
isopropylcyclopentane	Cycloalkanes
methane	Alkanes
methanethiol	Alkanethiols
methanol	Alkanols
methenamine	Cycloalkylamines
methyl formate	Esters
methyl 2-methylpropenoate	Esters
methyl nitrate	Alkyl Nitrates and Nitroalkanes
methylamine	Alkylamines
methylcyclobutane	Cycloalkanes
methylcyclohexane	Cycloalkanes
methylcyclopentane	Cycloalkanes
methylenecyclobutane	Cycloalkenes
methylethylamine	Alkylamines
methyloxacyclopropane	Oxacycloalkanes
N,*N*-dimethylaniline	Aromatic Amines
naphthalene	Aromatic Hydrocarbons
n-butane	Alkanes
n-butanoic acid	Carboxylic Acids
n-butylamine	Alkylamines
n-butylbenzene	Aromatic Hydrocarbons
n-decane	Alkanes
n-dodecane	Alkanes
neohexane	Alkanes

neopentane	Alkanes
n-heptane	Alkanes
n-hexadecane	Alkanes
n-hexane	Alkanes
nitrobenzene	Aromatic CHNOX
nitrogen	Nitrogen/Hydrogen
nitroglycerin	Alkyl Nitrates and Nitroalkanes
nitromethane	Alkyl Nitrates and Nitroalkanes
n-nonane	Alkanes
n-octane	Alkanes
n-pentane	Alkanes
n-propylbenzene	Aromatic Hydrocarbons
n-propylcyclopentane	Cycloalkanes
octamethylcyclotetrasiloxane	Siloxanes
oxirane	Oxacycloalkanes
oxygen	Hydrogen/Oxygen
pentachloroethane	Chloroalkanes
pentachlorophenol	Pentachorophenol
pentafluoroethane	Fluoroalkanes
pentanenitrile	Alkanenitriles
perylene	Polycyclic Aromatic Hydrocarbons
phenanthrene	Polycyclic Aromatic Hydrocarbons
phenol	Aromatic Alcohols
phosgene	Carbonyl Halides
piperidine	Cycloalkylamines
propanal	Aldehydes
propane	Alkanes
propanenitrile	Alkanenitriles
propanoic acid	Carboxylic Acids
propene	Alkenes
propenenitrile	Alkanenitriles
propylcyclohexane	Cycloalkanes
propyne	Alkynes
pyrene	Polycyclic Aromatic Hydrocarbons
pyrrole	Cycloalkylamines
ethenylbenzene	Aromatic Hydrocarbons
sucrose	Sugars and Ethanediol

tert-butanol	Alkanols
tert-butylamine	Alkylamines
tert-butylbenzene	Aromatic Hydrocarbons
tert-butylcyclohexane	Cycloalkanes
tetrabromomethane	Bromoalkanes
tetrachloroethene	Chloroalkenes
tetrachloromethane	Chloroalkanes
tetrafluoroethene	Fluoroalkenes
tetrafluoromethane	Fluoroalkanes
tetralin	Bicycloalkanes
tetranitromethane	Alkyl Nitrates and Nitroalkanes
thiacyclopentane	Sulfur-Substituted Cyclohydrocarbons
thiophene	Sulfur-Substituted Cyclohydrocarbons
toluene	Aromatic Hydrocarbons
trans-decalin	Bicycloalkanes
tribromofluoromethane	Bromofluoroalkanes
tribromomethane	Bromoalkanes
trichloroethene	Chloroalkenes
trichlorofluoromethane	Chlorofluoroalkanes
trichloromethane	Chloroalkanes
triethanolamine	Oxidized Nitrogen-Substituted Hydrocarbons
triethylamine	Alkylamines
trifluoroethene	Fluoroalkenes
trifluoromethane	Fluoroalkanes
trimethylamine	Alkylamines
trinitrotoluene	Aromatic CHNOX
urea	Oxidized Nitrogen-Substituted Hydrocarbons
vinyl acetate	Esters
water	Hydrogen/Oxygen

2. Normal Boiling Points T_b (P = 1 atm) and Melting Points T_m

2.1. Overview

In this section, we compiled, evaluated, and recommended normal boiling points T_b (P = 1 atm = 101.325 kPa) and normal melting points T_m of hydrocarbons, substituted hydrocarbons, and a few other compounds of physical, chemical, and engineering interest. (A few triple points and sublimation points are included). The substituted hydrocarbons include different classes of oxygen-, nitrogen-, sulfur-, and halogen-substituted hydrocarbons. We provide about 2000 normal boiling points, 100 melting points, for about 460 compounds from about 850 source references. All of these data are provided in Table 2-1. Although this is an extensive compilation, for some compounds, it is not comprehensive. All compounds, however, have a good selection of values from the literature, sufficient to provide an evaluated recommendation. The boiling points provided here were derived from direct boiling point, liquid-vapor equilibrium, vapor pressure determinations – and also from equation-of-state (EOS) formulations. The most accurate normal boiling points come from NIST TRC REFPROP[2018LEM] and NIST TRC TDE,[2019DIK] although for some compounds we did select other values. All values that were compiled are given in Table 2-1, while only the recommended values are provided in Table 2-2. All sources of data for the boiling and melting points that were compiled from the literature are given in the references.

We provide uncertainties from the original sources where available. The recommended values of boiling points provided here were selected from reliable original sources (not weighted averages). The uncertainties given here for the recommended values of the boiling points are generally expanded uncertainties at the 95 % confidence level (2σ, Type B).[1994TAY] The uncertainty column is identified with "unc", since many workers did not identify whether the uncertainties were 1σ or 2σ. All our recommended values are 2σ. The highest quality data are those derived from equation of state (EOS) formulations with about one half of these (excluding outliers) having very low expanded uncertainties of (0.01 to 0.06) K, and the other half having still low expanded uncertainties of (0.06 to 0.16) K. The expanded uncertainties (2σ) for the EOS predicted normal boiling points were derived from the reported standard uncertainties (1σ) in pressure and the temperature dependence of the pressure, $(1/P)\,(\partial P/\partial T)$. Vapor pressure determinations of boiling points are relatively accurate – but about half as accurate as those derived from EOS formulations. In many cases, we were able to assign an average uncertainty to each set of data from the measurements of individual research groups by comparing the deviations of their reported boiling points to other data in the literature, as well as considering reported uncertainties (1σ), when provided in the original sources. We estimated that about 45 % of these sets of boiling points had deviations of about (0.05 to 0.10) K, about 35 % had deviations of (0.10 to 0.25) K, about 15 % had deviations of (0.25 to 0.6) K, and about 5 % had deviations >0.6 K. For boiling points derived from other vapor pressure measurements, where there was insufficient data for sampling a set from a particular research group, we assigned a generic expanded uncertainty of U = 0.15 K, except in a few cases where we believed that it was higher. Vapor-liquid equilibrium determinations of boiling points are also relatively accurate –

we estimated that most of the boiling points had expanded uncertainties on the order of U = (0.15 to 0.25) K – roughly a median value. For direct determinations of boiling points, our analysis suggests that about 50 % of the values had expanded uncertainties of U = (0.05 to 0.20) K, 20 % with U = (0.2 to 0.5) K, 20 % with U = (0.5 to 1.0) K, and 10 % with U > 1 K. Where the boiling points were derived from direct boiling point measurements, we assigned expanded uncertainties based on the range of values (Type B uncertainties)[1994TAY] from many different determinations.

We also provide suggested melting points for compounds above 273 K (0 °C). These are important for determining enthalpies of combustion for some compounds which require enthalpies of melting or sublimation. We categorized the methods that were used to determine the boiling points and melting points reported in each of the sources, as best we could.

The overall procedure was that we first compiled values from the literature taking many from the NIST Chemistry Webbook, [2021LIN] and then selected recommended values for each compound. We then used the NIST TRC Thermodata Engine (TDE) [2021DIK] to independently screen our selections and make corrections as needed. In most cases, the values from TDE agreed with our selections within the uncertainties. A fraction of the uncertainties assigned by TDE (a semi-automated evaluation method) were either too small or too large relative to our assigned uncertainties. We investigated these differences and made corrections as needed. We then also used NIST TRC REFPROP[2018LEM] to screen our selections for boiling points – and almost always selected the recommended value from REFPROP, since they are derived from EOS formulations.

The columns labeled “Phase” and “TRS” indicate the phase and the type of the transition point, respectively. For compounds that are in the gas phase at room temperature, we have designated these as Phase=“gas” and transition point trs=”BP” to reflect this. For example, H_2 becomes a gas at T=20.369 K and a liquid below that temperature. We have also included triple points (trs=”TP”) for just a few compounds where the melting and triple points do not differ by much. The column labeled “SEL” indicates that data is a selected/recommended value. Those labeled “SEL” are the selected value at standard state (e.g., [*liq* → *gas*], where compound is a liquid at standard state), while those labeled “SEL1” or “SEL2” are for other states (e.g., [*sol* → *liquid*], melting [*sol* → *liquid*], or sublimation [*sol* → *gas*]). The column labeled “Method” provides an indication of the method used to determine the boiling point or melting point. A legend for the “Method” column is provided in Table 2-3.

In Tables 2-1 and 2-2, the compounds are arranged first by primary and secondary chemical class and then by molecular formula.

Primary and Secondary Chemical Class

1. **Small Molecules**
2. **Hydrogen/Oxygen**
   a. Nitrogen/Hydrogen
   b. Nitrogen/Oxygen
   c. Sulfur/Hydrogen/Oxygen
   d. Boron/Hydrogen/Oxygen
   e. Hydrogen Halides
3. **Hydrocarbons**
   a. Carbon
   b. Alkenes
   c. Alkadienes
   d. Alkynes
   e. Alkenynes
   f. Alkadiynes
   g. Cycloalkanes
   h. Cycloalkenes
   i. Cycloalkadienes
   j. Bicycloalkanes
4. **Aromatic Hydrocarbons**
   a. Alkylbenzenes
   b. Alkenylbenzenes
   c. Benzocycloalkanes
   d. Benzocycloalkenes
   e. Alkylnapthalenes
   f. Polycyclic Aromatics
5. **Oxidized Hydrocarbons**
   a. Carbon Oxides
   b. Alkanols
   c. Glycols
   d. Sugars
   e. Phenols
   f. Alkyl ethers
   g. Aldehydes
   h. Alkenals
   i. Ketones
   j. Carboxylic Acids
   k. Alkyl Esters
   l. Alkenyl Esters
   m. Alkanoic Anhydrides
   n. Oxacycloalkanes
   o. Oxacycloalkadienes
   p. Oxacycloketones
   q. Dioxanes and Trioxanes
   r. Furandione and D-Camphor
   s. Aromatic Alcohols
   t. Aromatic Aldehydes and Acids
6. **Nitrogen-Substituted Hydrocarbons**
   a. Hydrogen Cyanides
   b. Alkylamines
   c. Cycloalkylamines
   d. Azacycloalkanes
   e. Methenamines
   f. Azacycloalkadienes
   g. Alkanenitriles
   h. Alkenenitriles
   i. Cyanogens
   j. Alkylhydrazines
   k. Melamines
   l. Pyridines
   m. Anilines
   n. Oxidized Amines
   o. Alkyl Nitrates and Nitroalkanes
   p. Isocyanates
   q. Nitro Aromatics
7. **Sulfur-Substituted Hydrocarbons**
   a. Alkanethiols
   b. Alkyl Sulfides
   c. Thiacycloalkanes
   d. Thiacycloalkenes
   e. Aromatic Thiols
   f. Alkyl Sulfoxides
8. **Halogen-Substituted Hydrocarbons**
   a. Fluoroalkanes
   b. Fluoroalkenes
   c. Chloroalkanes
   d. Chloroalkenes
   e. Chloroacetylenes
   f. Chloroaromatics
   g. Bromoalkanes
   h. Bromoalkenes
   i. Iodoalkanes
   j. Chlorofluoromethanes
   k. Chlorofluoroethanes
   l. Chlorofluoroalkenes
   m. Bromofluoroalkanes
   n. Bromochloroalkanes
   o. Bromochlorofluoroalkanes
   p. Carbonyl Halides
   q. Chlorophenols
9. **Siloxanes**

2.2. Normal Melting and Boiling Points (Compilation)

All values that were compiled are given in Table 2-1, while only the recommended values are provided in Table 2-2, with all references for melting and boiling point data provided in the last subsection 2.4.

Table 2-2. Normal Melting and Boiling Points

Formula	Compound	Phase	SEL	trs	T_{trs}/K	unc/K	Method	Reference
SMALL MOLECULES								
Hydrogen/Oxygen								
H_2	hydrogen	gas	SEL	BP	20.369	0.014	EOS	2009LEA
				BP	20.369	0.014	EOS-rev	2018LEM
O_2	oxygen	gas	SEL	BP	90.188	0.029	EOS	1991STE
				BP	90.188	0.029	EOS-rev	2018LEM
H_2O	water	liq	SEL	BP	373.124	0.014	EOS	1995WAG
		sol	SEL1	MP	273.153	0.001	EOS	2006FEI
			SEL2	TP	273.16	0.01	DEF	1990PRE
		liq		BP	373.124	0.014	EOS-rev	2018LEM
H_2O_2	hydrogen peroxide	liq	SEL	BP	426.31	0.05	VLE rev	2004MAN
		sol	SEL1	MP	272.69	0.02	SLE	1951FOL
			SEL2	TP	272.74	0.05	TP	1954GIG
		liq		BP	426.2	1.2	BP rev	2019DIK
				BP	423.4		VLE Extrap	1952SCA
		sol		MP	273.2		MP	1954GIG
				MP	272.3		MP	1928CUT
				MP	271.5		MP	1920MAA
				TP	272.74	0.05	review	2019DIK
Nitrogen/Hydrogen								
N_2	nitrogen	gas	SEL	BP	77.355	0.007	EOS	2000SPA
				BP	77.355	0.007	EOS-rev	2018LEM
H_3N	ammonia	gas	SEL	BP	239.823	0.020	EOS	2018GAO
				BP	239.823	0.020	EOS-rev	2022LEM
				BP	239.8	0.3	VP rev	1947STU
H_4N_2	hydrazine	liq	SEL	BP	386.7	0.9	BP	1989TIP
				BP	387.227	0.015	BP rev	2019DIK
				BP	386.8	1.2	BP rev	2012KRO
				BP	387.3		BP	1934HIE

HN_3	hydrogen azide	liq	SEL	BP	308.9	1.5	BP rev	2007LID
Nitrogen/Oxygen								
N_2O	nitrous oxide	gas	SEL	BP	184.68	0.07	EOS	2006LEM
				BP	184.68	0.07	EOS-rev	2018LEM
ClH_4NO_4	ammonium perchlorate	sol	SEL	dec	595.9	4.0	DTA	2004LIU
			SEL	TP	513.2	1.0	TP rev	2019DIK
Sulfur/Hydrogen/Oxygen								
H_2S	hydrogen sulfide	gas	SEL	BP	212.85	0.10	EOS	2006LEM
				BP	212.85	0.10	EOS-rev	2018LEM
				BP	212.86	0.26	BP rev	2012KRO
				BP	218.9			2004SAK
				BP	212.87	0.10	EOS	1983GOO
				BP	212.60	0.18	VP rev	1947STU
O_2S	sulfur dioxide	gas	SEL	BP	263.14	0.09	EOS	2016GAO
				BP	263.14	0.09	EOS-rev	2018LEM
Boron/Hydrogen/Oxygen								
B_2H_6	diborane	gas	SEL	BP	180.6	0.1	VP	1959PAR
				BP	180.80	0.19	BP rev	2019DIK
				BP	180.80	0.19	VLE	2012KRO
				BP	180.7		VP	1961DIT
				BP	180.6			1956WIR
				BP	180.7			1956LAN
Hydrogen Halides								
ClH	hydrogen chloride	gas		BP	188.173	0.088	EOS	2018THO
				BP	188.173	0.088	EOS-rev	2018LEM
HYDROCARBONS								
Carbon								
C	graphite	sol	SEL	MP	4800	100	MP rev	2005SAV
				MP	4800	100	MP	2004BAS
				MP	4800	200	MP	2003KOR
				MP	4660		MP	2001KER
				MP	4750	150	MP	2000BAS
				MP	4800	150	MP	1998MUS
				MP	4900	200	MP	1993POT
				MP	4330	50	MP	1990CEZ
				MP	4700		MP	1988SHE
Alkanes								
CH_4	methane	gas	SEL	BP	111.667	0.013	EOS	1991SET

				BP	111.667	0.013	EOS-rev	2018LEM
				BP	111.7			2016HUR
				BP	111.67	0.22	BP rev	2012KRO
				BP	111.65	0.02		1976PAV
				BP	111.70	0.08	VP	1972PRY
C_2H_6	ethane	gas	SEL	BP	184.566	0.004	EOS	2006BUC
				BP	184.566	0.004	EOS-rev	2018LEM
				BP	184.6		BP comp	2016HUR
				BP	184.57	0.17	BP rev	2012KRO
				BP	184.6	0.2		1971STR
				BP	184.5	0.1		1964ZIE
				BP	184.10	0.15		1937WIT
				BP	184.9	0.5	VP	1928COF
				BP	184.48	0.10	VP	1926LOO
C_3H_8	propane	gas	SEL	BP	231.039	0.009	EOS	2009LEM
				BP	231.039	0.009	EOS-rev	2018LEM
				BP	231.1		BP comp	2016HUR
				BP	231.036	0.066	BP rev	2012KRO
				BP	231.07	0.08		1977GOO
				BP	231.1			1971STR
				BP	231.1		review	1948ROS
				BP	231.02	0.15	VP	1938KEM
				BP	228.7	0.5	VP	1928COF
C_4H_{10}	isobutane	gas	SEL	BP	261.40	0.26	EOS	2006BUC2
				BP	261.40	0.26	EOS-rev	2018LEM
				BP	261.4		BP comp	2016HUR
				BP	261.4	0.4	BP rev	2012KRO
				BP	261.13	0.15	VLE	1976STE
				BP	261.0	0.3	VLE	1973DAS
				BP	261.4	0.2	VLE	1967GIL
				BP	261.41	0.15	VP	1940AST1
				BP	263.0	0.5	VP	1928COF
	n-butane	gas	SEL	BP	272.66	0.12	EOS	2006BUC2
				BP	272.66	0.12	EOS-rev	2018LEM
				BP	272.7		BP comp	2016HUR
				BP	272.66	0.17	BP rev	2012KRO
				BP	272.64	0.08	VP	1982HAY
				BP	272.3	0.3	VLE	1973DAS2

				BP	272.7		VLE	1967GIL
				BP	272.77	0.15	VP	1940AST2
				BP	272.7	0.5	VP	1928COF
C_5H_{12}	isopentane	liq	SEL	BP	301.0	0.7	EOS	2006LEM
				BP	301.0	0.7	EOS-rev	2018LEM
				BP	300.98	0.15	BP rev	2012KRO
				BP	301.0	0.2	GLC	1957DES
				BP	301.00	0.18	VP rev	1947STU
				BP	301.05	0.15	BP rev	1947FEN
				BP	301.00	0.07	VP	1945WIL
	neopentane	gas	SEL	BP	282.650	0.028	EOS	2006LEM
				BP	282.665	0.019	BP rev	2019DIK
				BP	282.650	0.028	EOS-rev	2018LEM
				BP	282.655	0.093	BP rev	2012KRO
				BP	282.65	0.03	EOS	2006LEM
				BP	282.64	0.04	VP	1975HOP
				BP	282.65	0.06	VP ebul	1974OSB
				BP	282.7	0.2	GLC	1957DES
	n-pentane	liq	SEL	BP	309.21	0.12	EOS	2022THO
				BP	309.3		VLE	2021TSU
				BP	309.21	0.12	EOS-rev	2018LEM
				BP	309.2		BP comp	2016HUR
				BP	309.21	0.21	BP rev	2012KRO
				BP	309.22	0.06	VP ebul	1974OSB
				BP	309.2	0.2	GLC	1957DES
				BP	309.25	0.15	BP rev	1947FEN
C_6H_{14}	2,3-dimethylbutane	liq	SEL	BP	331.09	0.07	VP	1945WIL
				BP	331.12	0.09	BP rev	2019DIK
				BP	331.18	0.06	EOS-rev	2018LEM
				BP	331.2		VLE	1992HIA
				BP	331.3		VLE	1970KIR
				BP	331.0		VLE	1967MCC
				BP	331.4			1948RUS
				BP	331.10	0.15	BP rev	1947FEN
				BP	331.2		VLE	1946KAY
	3-methylpentane	liq	SEL	BP	336.43	0.07	VP	1945WIL
				BP	336.40	0.06	BP rev	2019DIK
				BP	336.402	0.055	BP rev	2012KRO

				BP	336.4	0.2	GLC	1957DES
				BP	336.30	0.15	BP rev	1947FEN
				BP	336.5	0.4	BP rev	1935LES
	isohexane	liq	SEL	BP	333.36	0.06	EOS	2006LEM
				BP	333.39	0.03	BP rev	2019DIK
				BP	333.36	0.06	EOS-rev	2018LEM
				BP	333.36	0.21	BP rev	2012KRO
				BP	333.36	0.06	EOS	2006LEM
				BP	334.4	0.3	VLE	1999LOR
				BP	333.40	0.15	BP rev	1947FEN
				BP	333.42	0.07	VP	1945WIL
	neohexane	liq	SEL	BP	322.85	0.13	EOS-rev	2018LEM
				BP	322.87	0.05	BP rev	2019DIK
				BP	322.85	0.13	EOS-rev	2018LEM
				BP	332.9	0.2	GLC	1957DES
				BP	322.80	0.15	BP rev	1947FEN
				BP	322.89	0.07	VP	1945WIL
	n-hexane	liq	SEL	BP	341.87	0.13	EOS	2022THO2
				BP	341.87	0.13	EOS-rev	2018LEM
				BP	341.9		BP comp	2016HUR
				BP	341.87	0.15	BP rev	2012KRO
				BP	342.0	0.1	VLE	1998FEN
				BP	341.85	0.15	BP rev	1947FEN
				BP	341.89	0.07	VP	1945WIL
				BP	341.9		BP rev	1935LES
C_7H_{16}	2,2,3-trimethylbutane	liq	SEL	BP	354.03	0.10	VP	1949FOR
				BP	353.99	0.09	BP rev	2019DIK
				BP	354.0	0.2	GLC	1957DES
				BP	354.2		VLE	1949DEN
				BP	354.05	0.15	BP rev	1947FEN
				BP	354.0			1943MCA
				BP	353.9		BP rev	1922TIM
	2,3-dimethylpentane	liq	SEL	BP	362.93	0.06	VLE	1974OSB
				BP	362.9	0.4	BP rev	2019DIK
				BP	363.0		VLE	1999MON
				BP	363.3		VLE	1960KYL
				BP	363.0	0.2	GLC	1957DES
				BP	362.93	0.10	VP	1949FOR

				BP	362.90	0.15	BP rev	1947FEN
	2,4-dimethylpentane	liq	SEL	BP	353.7	0.3	VLE	1976TRI
				BP	353.6	0.3	BP rev	2019DIK
	3,3-dimethylpentane	liq	SEL	BP	359.21	0.10	VP	1949FOR
				BP	359.19	0.08	BP rev	2019DIK
				BP	359.25	0.15	BP rev	1947FEN
	3-methylhexane	liq	SEL	BP	365.00	0.10	VP	1949FOR
				BP	364.9	0.4	BP rev	2019DIK
				BP	365.00	0.15	BP rev	1947FEN
	isoheptane	liq	SEL	BP	363.20	0.15	VP	1949FOR
				BP	363.1	0.4	BP rev	2019DIK
				BP	363.20	0.15	BP rev	1947FEN
	neoheptane	liq	SEL	BP	352.25	0.15	BP rev	1947FEN
				BP	352.33	0.06	BP rev	2019DIK
				BP	352.1		BP rev	1935LES
	n-heptane	liq	SEL	BP	371.55	0.07	EOS	2018TEN
				BP	371.55	0.07	EOS-rev	2018LEM
				BP	371.6		BP comp	2016HUR
				BP	371.53	0.29	BP rev	2012KRO
				BP	371.5	0.1	VLE	1995WIS
				BP	371.51	0.07		1954DOU
				BP	371.55	0.15	BP rev	1947FEN
				BP	371.58	0.07	VP	1945WIL
				BP	371.6		BP rev	1935LES
C_8H_{18}	2,2,4-trimethylpentane	liq	SEL	BP	372.36	0.14	EOS	2018BLA
				BP	372.36	0.14	EOS-rev	2018LEM
				BP	390.9		BP comp	2016HUR
				BP	372.4	0.1	BP rev	2012KRO
				BP	372.4	0.2	VLE	1995HIA2
				BP	372.39	0.07	VP	1945WIL
	2,2-dimethylhexane	liq	SEL	BP	379.74	0.07	VP	1945WIL
				BP	379.967	0.014	BP rev	2019DIK
				BP	379.99	0.15	GLC	1957DES
				BP	380.2			1951AUD
				BP	379.7			1948BUC
				BP	379.77	0.18	VP rev	1947STU
				BP	380.05	0.15	BP rev	1947FEN
				BP	379.97	0.10	BP	1946FOR

				BP	380.3			1945HER
	2-methylheptane	liq	SEL	BP	390.90	0.15	BP rev	1947FEN
				BP	390.78	0.09	BP rev	2019DIK
				BP	390.8	0.2	BP rev	1957DES
				BP	390.4		BP rev	1935LES
	n-octane	liq	SEL	BP	398.79	0.14	EOS	2018BEC
				BP	398.79	0.14	EOS-rev	2022LEM
				BP	398.8		BP comp	2016HUR
				BP	398.9		VLE	2013FER
				BP	398.77	0.28	BP rev	2012KRO
				BP	399.2		VLE	2007RED
				BP	399.2		VLE	2006SUR
				BP	398.8		VLE	2000HIA
				BP	398.6		VLE	1999WIS
				BP	398.8	0.2	VLE	1995HIA2
				BP	398.8		VLE	1995HIA
				BP	398.7		VLE	1986PAU
				BP	398.8		VLE	1982RED
				BP	398.75	0.20	VLE	1976RAD
				BP	398.75	0.15	BP rev	1947FEN
				BP	398.82	0.07	VP	1945WIL
				BP	398.6		BP rev	1935LES
C_9H_{20}	isononane	liq	SEL	BP	416.41	0.15		1950MEA
				BP	416.4	1.3	BP rev	2019DIK
				BP	416.1	0.3	BP rev	1950MEA
				BP	416.5	0.3	BP rev	1948ROS
				BP	416.41	0.15	BP rev	1947FEN
				BP	416.0		BP rev	1935LES
	neononane	liq	SEL	BP	403.65	0.15	BP rev	1947FEN
				BP	405.6	2.2	BP rev	2019DIK
	n-nonane	liq	SEL	BP	423.91	0.15	EOS	2006LEM
				BP	423.91	0.15	EOS-rev	2018LEM
				BP	424.0		BP comp	2016HUR
				BP	423.91	0.17	BP rev	2012KRO
				BP	423.82	0.25		1982RED
				BP	423.95	0.10	VP	1949FOR
				BP	423.95	0.15	BP rev	1947FEN
$C_{10}H_{22}$	*n*-decane	liq	SEL	BP	447.27	0.16	EOS	2006LEM

				BP	447.27	0.16	EOS-rev	2018LEM
				BP	447.27	0.14	BP rev	2012KRO
				BP	447.3	0.1	VP	1988GIE
				BP	447.3	0.2	GLC	1957DES
				BP	447.4	0.3		1955HAN
				BP	447.20	0.15	BP rev	1947FEN
				BP	447.27	0.07	VP	1945WIL
$C_{11}H_{24}$	*n*-undecane	liq	SEL	BP	469.05	0.15	BP rev	1947FEN
				BP	469.04	0.19	BP rev	2019DIK
$C_{12}H_{26}$	*n*-dodecane	liq	SEL	BP	489.44	0.08	EOS	2004LEM
		sol	SEL1	MP	263.5	0.2	MP	1983OTT
			SEL2	TP	263.6		EOS	2004LEM
		liq		BP	489.4	0.3	BP rev	2019DIK
				BP	489.44	0.08	EOS-rev	2018LEM
				BP	489.41	0.15	BP rev	1947FEN
		sol		TP	263.6		EOS-rev	2018LEM
$C_{16}H_{34}$	*n*-hexadecane	liq	SEL	BP	559.9	0.2		2018LEM
		sol	SEL1	MP	291.3	0.1	MP	1986SNO
			SEL2	TP	291.3			2018LEM
		liq		BP	560.1	1.5	BP rev	2019DIK
				BP	560.5	0.6	VP	2014SII
				BP	560.2			1989CRC
				BP	559.9	0.2	VP	1954CAM
				BP	559	2		1950MUM
				BP	559.2		BP rev	1949BOO
Alkenes								
C_2H_4	ethene	gas	SEL	BP	169.38	0.02	EOS	2000SMU
				BP	169.38	0.02	EOS-rev	2018LEM
				BP	169.4		BP comp	2016HUR
				BP	169.38	0.12	BP rev	2012KRO
				BP	169.35	0.02		1986JAH
				BP	169.37	0.03	VP	1950MIC
				BP	169.9	0.2	VP	1940LAM
				BP	169.3	0.5	VP	1928COF
C_3H_6	propene	gas	SEL	BP	225.53	0.04	EOS-rev	2018LEM
				BP	225.53	0.04	EOS	2022LEM
				BP	225.5		BP comp	2016HUR
				BP	225.5	0.4	BP rev	2012KRO

				BP	225.5	0.4		1946MOR
				BP	225.9	0.2	VP	1940LAM
				BP	225.38	0.15	VP	1939POW
				BP	226.2	0.5	VP	1928COF
C_4H_8	1-butene	gas	SEL	BP	266.83	0.15	VLE	1976STE
				BP	266.82	0.29	BP rev	2019DIK
				BP	266.84	0.06	EOS-rev	2018LEM
				BP	267.0		BP comp	2016HUR
				BP	266.84	0.24	BP rev	2012KRO
				BP	266.9	0.2		1949FOE
				BP	266.9		BP	1946MOR
				BP	267.24	0.11	VP	1940LAM
				BP	266.6		BP	1930LUC
				BP	267.4	0.5	VP	1928COF
	2-butene, (*E*)-	gas	SEL	BP	274.01	0.15	VP	1945GUT
				BP	274.03	0.11	BP rev	2019DIK
				BP	274.03	0.08	EOS-rev	2018LEM
				BP	274.03	0.09	BP rev	2012KRO
				BP	274.03	0.08	EOS	2005LEM
				BP	274.44	0.07	VP	1940LAM
				BP	274.11	0.15		1937CAR
				BP	274.2	0.5	VP	1928COF
	2-butene, (*Z*)-	gas	SEL	BP	276.87	0.08	VP	1944SCO
				BP	276.83	0.10	BP rev	2019DIK
				BP	276.87	0.05	EOS-rev	2018LEM
				BP	276.87	0.08	BP rev	2012KRO
				BP	276.87	0.05	EOS	2005LEM
				BP	276.9	0.5		1949FOE
				BP	277.07	0.14	VP	1940LAM
	isobutene	gas	SEL	BP	266.05	0.15	VP	1940LAM
				BP	266.17	0.29	BP rev	2019DIK
				BP	266.15	0.13	EOS-rev	2018LEM
				BP	266.2	0.2	BP rev	2012KRO
				BP	266.15	0.13	EOS	2005LEM
				BP	266.4	0.5		1949FOE
				BP	266.6	0.5	VP	1928COF
C_5H_{10}	1-pentene	liq	SEL	BP	303.12	0.08	VP	1949SCO
				BP	303.10	0.07	BP rev	2019DIK

				BP	303.10	0.01	EOS-rev	2018LEM
				BP	303.2		BP comp	2016HUR
				BP	303.11	0.07	BP rev	2012KRO
				BP	303.22	0.04		1951DAY
				BP	303.12	0.06	VP	1950FOR
				BP	303.15	0.15	BP rev	1947FEN
	2-methyl-1-butene	liq	SEL	BP	304.30	0.13	VP	1949SCO
				BP	304.25	0.21	BP rev	2019DIK
				BP	304.3	0.2	BP rev	2012KRO
				BP	304.3	0.2	GLC	1957DES
				BP	304.20	0.15	BP rev	1947FEN
	2-methyl-2-butene	liq	SEL	BP	311.72	0.15	VP	1949SCO
				BP	311.70	0.28	BP rev	2019DIK
				BP	311.7	0.2	GLC	1957DES
				BP	311.9	0.2	VP	1940LAM
	2-pentene, (*E*)-	liq	SEL	BP	309.51	0.08	VP	1950SCO2
				BP	309.48	0.03	BP rev	2019DIK
				BP	309.476	0.036	BP rev	2012KRO
				BP	309.0			1948THO
				BP	309.5		VLE	1946GER
				BP	309.0		VLE	1941EWE
				BP	309.4			1937CAR
	2-pentene, (*Z*)-	liq	SEL	BP	310.09	0.08	VP	1950SCO2
				BP	310.07	0.03	BP rev	2019DIK
				BP	310.076	0.035	BP rev	2012KRO
				BP	310.0			1951HOF
				BP	310.2			1948THO
				BP	309.7			1937CAR
	3-methyl-1-butene	gas	SEL	BP	293.21	0.08	VP	1950SCO2
				BP	293.21	0.04	BP rev	2019DIK
				BP	293.201	0.034	BP rev	2012KRO
				BP	293.2	0.5		1946GER
C_6H_{12}	1-hexene	liq	SEL	BP	336.64	0.06	VP	1950FOR
				BP	336.60	0.08	BP rev	2019DIK
				BP	336.7		BP comp	2016HUR
				BP	336.58	0.08	BP rev	2012KRO
				BP	336.7	0.2	VLE	1966SUR
				BP	336.6	0.2	GLC	1957DES

C_7H_{14}	1-heptene	liq	SEL	BP	366.71	0.06	VP	1950FOR
				BP	366.77	0.09	BP rev	2019DIK
				BP	366.8		BP comp	2016HUR
				BP	366.76	0.07	BP rev	2012KRO
				BP	366.7	0.8		1965KAA
				BP	366.80	0.15	BP rev	1947FEN
				BP	363.4			1935MUL
C_8H_{16}	1-octene	liq	SEL	BP	394.43	0.06	VP	1950FOR
				BP	394.42	0.10	BP rev	2019DIK
				BP	394.5		BP comp	2016HUR
				BP	394.4	0.1	BP rev	2012KRO
				BP	394.4	0.2	GLC	1957DES
				BP	394.40	0.15	BP rev	1947FEN
C_9H_{18}	1-nonene	liq	SEL	BP	420.02	0.06	VP	1950FOR
				BP	420.01	0.06	BP rev	2019DIK
				BP	418.1			1957LOE
				BP	418.5			1931WIL
$C_{10}H_{20}$	1-decene	liq	SEL	BP	443.72	0.06	VP	1950FOR
				BP	443.72	0.09	BP rev	2019DIK
				BP	443.8			1950MEA
				BP	443.8			1935MUL
Alkadienes								
C_3H_4	allene	gas	SEL	BP	238.3	0.5	VP rev	1947STU
				BP	238.2	0.6	BP rev	2019DIK
				BP	240.9	0.3	EOS-rev	2018LEM
				BP	238.6		BP comp	2016HUR
				BP	239.0	0.5	BP rev	2012KRO
				BP	237.7			1956BLO
				BP	238.7	0.4		1954POM
				BP	240.0	0.2	VP	1940LAM
				BP	238.15	0.15	VP	1930LIV
				BP	241.2			1905LES
C_4H_6	1,2-butadiene	gas	SEL	BP	284.1	0.4		1946STR
				BP	284.00	0.17	BP rev	2019DIK
				BP	284.0		BP comp	2016HUR
				BP	284.1	0.4	eval	2012KRO
				BP	284.0		eval	1985MAJ
				BP	291.9	1.0	VP rev	1947STU

				BP	283.6			1947AST
				BP	283.5			1931HUR
	1,3-butadiene	gas	SEL	BP	268.44	0.15	VLE	1976STE
				BP	268.59	0.19	BP rev	2019DIK
				BP	268.8		BP comp	2016HUR
				BP	268.60	0.17	BP rev	2012KRO
				BP	268.7	0.4		1949FOE
				BP	268.62	0.15	VP	1933HEI
C_5H_8	1,2-pentadiene	liq	SEL	BP	318.01	0.06	VP	1950FOR
				BP	318	2		2021FIS
				BP	317.99	0.03	BP rev	2019DIK
				BP	318.1		BP comp	2016HUR
				BP	317.6	2.1	BP rev	2012KRO
				BP	318.80	0.06	VP ebul	1969OSB
	1,3-pentadiene	liq	SEL	BP	314.9	1.5		1956BUS
				BP	315.4	2.0	BP rev	2019DIK
				BP	315.3	1.7	BP rev	2012KRO
				BP	315.4	0.5	VP rev	1947STU
				BP	315.3			1935MUL
	1,4-pentadiene	liq	SEL	BP	299.12	0.15	VP	1950FOR
				BP	299.10	0.03	BP rev	2019DIK
				BP	299.10	0.04	BP rev	2012KRO
				BP	298.93	0.06	VP extrap	1969OSB
				BP	299.3	0.6		1949ELS
				BP	298.90	0.12	VP	1940LAM
	2-methyl-1,3-butadiene	liq	SEL	BP	307.19	0.15	VLE	1985HOW
				BP	307.20	0.06	BP rev	2019DIK
				BP	307.20	0.06	BP rev	2012KRO
				BP	307.26	0.08	VP	1964GUB
				BP	307.30	0.15		1963LE
				BP	307.0	0.6		1952GIL
				BP	307.2	0.5		1949FOE
Alkynes								
C_2H_2	acetylene	gas	SEL	BP	188.26	0.15	EOS-rev	2018LEM
		sol	SEL1	TP	191.75	0.15	EOS-rev	2018LEM
		gas		BP	188.8	0.5	VP extrap	2019DIK
				BP	188.5		sub rev	2013HAY
				BP	189.0		BP rev	1982BUC

				BP	188.41	0.10	sub VP	1956AMB
				BP	189.1		sub VP	1952ROB
				BP	189.1	0.5	sub VP	1950CLA
				BP	189.6		sub VP	1921MAA
				BP	189.1		sub VP	1915BUR
		sol		TP	192.0		sub rev	2019DIK
C_3H_4	propyne	gas	SEL	BP	249.80	0.15	VP	1967VAN
				BP	249.92	0.16	BP rev	2019DIK
				BP	250		EOS-rev	2018LEM
				BP	249.9		BP comp	2016HUR
				BP	248	15	BP rev	2012KRO
				BP	250		EOS	1992POL
				BP	249.9	1.0		1950RIC
				BP	245.4		VP	1921MAA
				BP	249.7			1905LES
		sol		TP	170.5		EOS-rev	2018LEM
				TP	170.5		EOS	1992POL
C_4H_6	1-butyne	gas	SEL	BP	281.18	0.15	VP	1950AST
				BP	281.21	0.06	BP rev	2019DIK
				BP	281.23	0.05	EOS-rev	2018LEM
				BP	281.22	0.14	BP rev	2012KRO
				BP	281.9		VLE	1952ROB
				BP	281.3	0.3		1947BOO
				BP	281.3		VP rev	1947API
				BP	281.3			1946STR
	2-butyne	liq	SEL	BP	300.1	0.2		1954POM2
				BP	300.106	0.012	BP rev	2019DIK
				BP	300.9	0.7	BP rev	2012KRO
				BP	300.1		BP	1945HEN
				BP	299.8			1939CON
C_5H_8	1-pentyne	liq	SEL	BP	313.5	0.3	VLE	2021TSU
				BP	313.0	1.3	BP rev	2019DIK
				BP	313	1	BP rev	2012KRO
				BP	313.4			1954POM2
				BP	313.4		BP	1945HEN
	2-pentyne	liq	SEL	BP	329.3	0.2		1954POM2
				BP	328.9	1.7	BP rev	2019DIK
				BP	328.9	1.3	BP rev	2012KRO

				BP	329.2			1954MIL
				BP	329.2		BP	1945HEN
C_6H_{10}	1-hexyne	liq	SEL	BP	344.5	0.2	VLE	2021TSU
				BP	344.32	0.16	BP rev	2019DIK
				BP	344.28	0.15	BP rev	2012KRO
				BP	344.5			1954POM2
				BP	344.6		BP	1945HEN
	2-hexyne	liq	SEL	BP	357.6	0.2	VLE	2021TSU
				BP	357.25	0.17	BP rev	2019DIK
				BP	357.5	0.2	BP rev	2012KRO
				BP	357.7			1954POM2
	3-hexyne	liq	SEL	BP	354.6	0.3		1954POM2
				BP	354.07	0.21	BP rev	2019DIK
				BP	354.7	0.5	BP rev	2012KRO
				BP	356.3	0.5	VP	1965RON
				BP	354.4			1955LEM
				BP	354.4			1954MIL
C_7H_{12}	1-heptyne	liq	SEL	BP	372.9	0.3	BP	1945HEN
				BP	372.93	0.16	BP rev	2019DIK
				BP	372.7		VLE	1948HEN
C_8H_{14}	1-octyne	liq	SEL	BP	399.4	0.3	BP	1945HEN
				BP	399.38	0.06	BP rev	2019DIK
Alkenynes								
C_4H_4	butenyne	gas	SEL	BP	276.2	2.0		1954HEN
				BP	279.2	1.3	BP rev	2019DIK
				BP	278.3		BP comp	2016HUR
				BP	279.2	1.0	BP rev	2012KRO
				BP	278.5	0.5	VP rev	1947STU
C_5H_6	1-penten-3-yne	liq	SEL	BP	332.4			1933JAC
				BP	332	4		2019DIK
	3-penten-1-yne	liq	SEL	BP	317.1	3.0		1954POM2
				BP	319	5	BP est	2019DIK
				BP	319	4	BP rev	2012KRO
				BP	320.2			1957PET
Alkadiynes								
C_4H_2	butadiyne	gas	SEL	BP	283.7	1.0		1954POM2
				BP	282.9	1.0	BP rev	2019DIK
				BP	283.5		BP comp	2016HUR

				BP	284.1	2.8	BP rev	2012KRO
				BP	282.5	0.5	VP rev	1947STU
Cycloalkanes								
C_3H_6	cyclopropane	gas	SEL	BP	241.7	0.4	EOS	1992POL
				BP	240.30	0.08	BP rev	2019DIK
				BP	241.7	0.4	EOS-rev	1998LEM
				BP	240.3		BP comp	2016HUR
				BP	242	7	BP rev	2012KRO
				BP	239.8	1.0	VP extrap	1962HAS
				BP	241.7		VP	1955GRA
				BP	239.7		VP	1947STU
				BP	240.27	0.15	VP	1946RUE1
				BP	240.5	0.5		1939GRO
				BP	240.3			1936HAS
				BP	240.1		VP	1934KOH
C_4H_8	cyclobutane	gas	SEL	BP	285.6	0.2	VP	1953RAT
				BP	285.7	0.4	BP rev	2019DIK
				BP	286.1		BP comp	2016HUR
				BP	285.7	0.4	BP rev	2012KRO
				BP	285.3			1953RAT
				BP	285.7			1952KAA
				BP	285.7	0.4		1949ROB
				BP	284.5			1949CAS
C_5H_{10}	cyclopentane	liq	SEL	BP	322.40	0.06	EOS	2015GED
				BP	322.40	0.06	EOS-rev	2018LEM
				BP	322.5		BP comp	2016HUR
				BP	322.40	0.09	BP rev	2012KRO
				BP	322.4		VLE	1978SEV
				BP	322.4	0.2	GLC	1957DES
				BP	322.5		VLE	1956MYE
				BP	322.40	0.15		1949FOE
				BP	322.5		VLE	1949DEN
				BP	322.35	0.15		1947FEN
				BP	322.41	0.07	VP	1945WIL
	methylcyclobutane	liq	SEL	BP	310	2		1953PIN
				BP	310	4	BP rev	2019DIK
				BP	310	3	BP rev	2012KRO
				BP	309.5			1937GRO

C_6H_{12}	cyclohexane	liq	SEL	BP	353.87	0.03	EOS	2014ZHO
				BP	353.865	0.017	EOS-rev	2018LEM
				BP	353.9		BP comp	2016HUR
				BP	353.86	0.17	EOS	2014ZHO
				BP	353.89	0.27	BP rev	2012KRO
				BP	353.90	0.15	VLE	1998FEN
				BP	353.8		VLE	1995WIS
				BP	354.0		VLE	1994TOJ
				BP	353.7		VLE	1989RAM
				BP	353.9		VLE	1989MAT
				BP	354.04	0.15	VP	1974KER
				BP	363.82	0.03	VLE	1973MAT
				BP	353.90	0.15	VLE	1965MAR
				BP	353.9	0.2	GLC	1957DES
				BP	353.85	0.15	BP rev	1947FEN
				BP	353.89	0.07	VP	1945WIL
	methylcyclopentane	liq	SEL	BP	344.96	0.07	VP	1945WIL
				BP	344.94	0.06	BP rev	2019DIK
				BP	344.937	0.061	BP rev	2012KRO
				BP	344.75	0.04	VP rev	1979KUD
				BP	344.97	0.15	VLE	1970WEA
				BP	345.0		VLE	1962KAE
				BP	345.0		VLE	1961BEL
				BP	345.0	0.2	GLC	1957DES
				BP	345.00	0.15		1949FOE
				BP	345.0		VLE	1949DEN
				BP	344.95	0.15	BP rev	1947FEN
				BP	344.8		BP	1945CRA
				BP	345.0		BP rev	1935LES
C_7H_{14}	1,1-dimethylcyclopentane	liq	SEL	BP	360.99	0.10	VP	1949FOR
				BP	361.0	0.3	BP rev	2019DIK
				BP	361.1		VLE	1949DEN
				BP	360.65	0.15	BP rev	1947FEN
	cycloheptane	liq	SEL	BP	391.92	0.08	VP	1956FIN
				BP	391.94	0.08	BP rev	2019DIK
				BP	391.7		BP rev	1989WEA
				BP	393.0			1986FIS
				BP	391.5			1976MEY

				BP	392.6			1965MUE
				BP	392.1	0.2	GLC	1957DES
				BP	392.0		VP rev	1954API
				BP	391.6			1952KAA
				BP	391.3		BP rev	1935LES
	ethylcyclopentane	liq	SEL	BP	376.61	0.10	VP	1949FOR
				BP	376.6	0.3	BP rev	2019DIK
				BP	376.60	0.15	BP rev	1947FEN
				BP	376.9		BP	1945CRA
	methylcyclohexane	liq	SEL	BP	374.12	0.15	VLE	1991AIZ
				BP	374.04	0.09	BP rev	2019DIK
				BP	374.0		EOS-rev	2018LEM
				BP	374.01	0.11	BP rev	2012KRO
				BP	374.1		VLE	1977WIS
				BP	373.9			1974RAO
				BP	373.9		VLE	1973WAD
				BP	374.1		VLE	1973NAG
				BP	374.1		VLE	1973CHI
				BP	374.0		VLE	1969RAJ
				BP	374.1	0.2	GLC	1957DES
				BP	374.08	0.07	VP	1945WIL
				BP	374.0		BP rev	1935LES
C_8H_{16}	ethylcyclohexane	liq	SEL	BP	405.05	0.15	BP rev	1935LES
				BP	404.92	0.03	BP rev	2019DIK
	isopropylcyclopentane	liq	SEL	BP	399.57	0.06	VP	1949FOR
				BP	399.544	0.022	BP rev	2019DIK
				BP	399.70	0.15		1949FOE
				BP	399.55	0.15	BP rev	1947FEN
				BP	399.6		BP	1945CRA
	n-propylcyclopentane	liq	SEL	BP	404.10	0.06	VP	1949FOR
				BP	404.07	0.07	BP rev	2019DIK
				BP	404.1	0.2	GLC	1957DES
				BP	404.1			1956EPS
				BP	404.20	0.15		1949FOE
				BP	404.1		BP rev	1949BOO2
				BP	404.15	0.15	BP rev	1947FEN
				BP	404.0		BP	1945CRA
				BP	404.5		BP rev	1935LES

C_9H_{18}	isopropylcyclohexane	liq	SEL	BP	427.71	0.10	VP	1949FOR
				BP	427.62	0.20	BP rev	2019DIK
				BP	427.8		BP rev	1945SMI
				BP	427.7		VLE	1938SMI
	propylcyclohexane	liq	SEL	BP	429.87	0.10	VP	1949FOR
				BP	429.85	0.08	BP rev	2019DIK
				BP	429.7		VLE	1950CHI
				BP	429.8		BP rev	1946BOO
				BP	429.9		BP rev	1945SMI
$C_{10}H_{20}$	1,3-diethylcyclohexane	liq	SEL	BP	445.7	1.5		1962ALL
				BP	447.1	2.4	BP rev	2019DIK
				BP	447.2		BP	1933SIG
	isobutylcyclohexane	liq	SEL	BP	444.47	0.07	VP	1949FOR
				BP	444.46	0.13	BP rev	2019DIK
				BP	444.4			1949BOO2
	tert-butylcyclohexane	liq	SEL	BP	444.74	0.10	VP	1949FOR
				BP	444.71	0.16	BP rev	2019DIK
				BP	444.9		BP rev	1945SMI
				BP	444.7		BP rev	1944BOO
Cycloalkenes								
C_3H_4	cyclopropene	gas	SEL	BP	237.6	1.5	BP	1941SCH
				BP	237.7	1.3	BP rev	2019DIK
				BP	237.6	1.3	BP rev	2012KRO
C_4H_6	cyclobutene	gas	SEL	BP	275.74	0.15	VP	1941HEI
				BP	275.70	0.20	BP rev	2019DIK
				BP	275.7	0.5	EOS-rev	2018LEM
				BP	275.2		BP rev	1989WEA
C_5H_8	cyclopentene	liq	SEL	BP	317.39	0.06	VP	1950FOR
				BP	317.4	0.1	VLE	2021TSU
				BP	317.37	0.04	BP rev	2019DIK
				BP	317.37	0.05	BP rev	2012KRO
				BP	317.6			1955TIM
				BP	317.40	0.15		1949FOE
				BP	317.6			1948ROB
				BP	317.2			1938CAR
				BP	317.5		VP	1937MAE
	methylenecyclobutane	liq	SEL	BP	315.35	0.15	BP rev	1947FEN
				BP	315	5	BP est	2019DIK

				BP	315	4	BP rev	2012KRO
				BP	315.0	0.5		1955CRI
				BP	314.9			1949ROB
				BP	315.4			1946SLA
C_6H_{10}	3-methylcyclopentene	liq	SEL	BP	338	1	BP	1945CRA
				BP	338.3	2.2	BP rev	2019DIK
				BP	338.1			1948ADK
				BP	338.35	0.15	BP rev	1947FEN
	cyclohexene	liq	SEL	BP	356.10	0.04	VP	1973MEY
				BP	356.07	0.08	BP rev	2019DIK
				BP	356.0		BP comp	2016HUR
				BP	353.89	0.27	BP rev	2012KRO
				BP	356.2		VLE	1989MAT
				BP	356.1	0.2	GLC	1957DES
				BP	356.2			1955TIM
				BP	356.13	0.06	VP	1950FOR
C_7H_{12}	1-ethylcyclopentene	liq	SEL	BP	379.6	0.2		1959PIN
				BP	379.31	0.08	BP rev	2019DIK
				BP	379.6			1965SAM
				BP	379.7			1958TUR
				BP	380.5			1952VAN
				BP	377			1948ADK
				BP	379.5		VP rev	1946API
				BP	379.7		BP rev	1935LES
	1-methylcyclohexene	liq	SEL	BP	383.42	0.15	VP	1960CAM
				BP	383.35	0.12	BP rev	2019DIK
				BP	383.3		VLE	1999BEV
				BP	383.1			1965SAM
				BP	382.7		BP	1958TUR
				BP	382.7		BP	1933SIG
	3-ethylcyclopentene	liq	SEL	BP	371.3		BP	1945CRA
				BP	371.0	3.3	BP rev	2019DIK
	cycloheptene	liq	SEL	BP	386.1	0.5	GLC	1958TUR
				BP	386.4	3.5	BP rev	2019DIK
				BP	388.1	0.2	GLC	1957DES
				BP	385.6			1956TRA
				BP	386.1			1954DOE
				BP	385.6			1953OWE

	methylenecyclohexane	liq	SEL	BP	376.58	0.04	VP	1973MEY
				BP	376.553	0.024	BP rev	2019DIK
				BP	376.55	0.03	BP rev	2012KRO
				BP	375.7		BP	1958TUR
				BP	375.4		BP	1956COP
				BP	376			1956CHI
				BP	356			1952STE
				BP	375.1			1952GOE
C_8H_{14}	1,2-dimethylcyclohexene	liq	SEL	BP	409	2	BP	1938CHI
				BP	410	3	BP est	2019DIK
				BP	408.9		BP	1933SIG
	1-ethylcyclohexene	liq	SEL	BP	410.11	0.05	VP	1960CAM
				BP	410.126	0.026	BP rev	2019DIK
				BP	408.4		BP	1965SAM
				BP	409.9		BP	1962COP
				BP	409	1		1958TUR
				BP	409.4		BP	1933SIG
Cycloalkadienes								
C_4H_4	cyclobutadiene	gas	SEL	BP	286	12	BP est	2019DIK
C_5H_6	1,3-cyclopentadiene	liq	SEL	BP	313.4	0.2	VP	1965HUL
				BP	313.34	0.07	BP rev	2019DIK
				BP	313.6	1.3	BP rev	2012KRO
				BP	314.7	0.5	VLE	1967LES
				BP	314.2	0.5	GLC	1957DES
				BP	313.9			1949MUR
				BP	313.2			1941BRO
				BP	313.3		BP	1936KIS
C_6H_8	1,3-cyclohexadiene	liq	SEL	BP	353.49	0.04	VP	1973MEY
				BP	353.475	0.022	BP rev	2019DIK
				BP	353.48	0.05	BP rev	2012KRO
				BP	353.44	0.10	VP	1989STE
				BP	353.53	0.10	VP	1973MEY
				BP	354.2	0.2	GLC	1957DES
				BP	353			1951BLO
				BP	353.7			1940WHI
	1,4-cyclohexadiene	liq	SEL	BP	362.66	0.05		1989STE
				BP	362.664	0.021	BP rev	2019DIK
				BP	362.67	0.04	BP rev	2012KRO

				BP	362.7		VP rev	1962API
C_8H_{12}	1,5-cyclooctadiene	liq	SEL	BP	421.8	2.0		1985TAS
				BP	424.0		VLE	2021TSU
				BP	418.8	2.7	BP est	2019DIK
Bicycloalkanes								
$C_{10}H_{18}$	*cis*-decalin	liq	SEL	BP	468.93	0.10	VP	1955CAM
				BP	468.94	0.14	BP rev	2019DIK
				BP	468.97	0.15	BP rev	2012KRO
				BP	468.70	0.15		1949FOE
				BP	468.9			1949BOO
	trans-decalin	liq	SEL	BP	460.42	0.10	VP	1955CAM
				BP	460.41	0.21	BP rev	2019DIK
				BP	460.41	0.25	BP rev	2012KRO
				BP	462.90	0.15		1949FOE
$C_{12}H_{22}$	cyclohexylcyclohexane	liq	SEL	BP	511.1	0.3	VP	1980WIE
		sol	SEL1	MP	277.2	0.5	MP	1983O'R
		liq		BP	511.2			2021EPA
				BP	510.89	0.25	BP rev	2019DIK
				BP	509.2		BP comp	2016HUR
				BP	510.92	0.25	BP rev	2012KRO
				BP	512.2	0.3	BP	1963MEA
				BP	512.2	0.4	VLE	1961JES
				BP	511.35	0.15	VP	1955MYE
				BP	512.0	0.3		1951WIS
				BP	510.2		BP	1933SIG

AROMATIC HYDROCARBONS								
Alkylbenzenes								
C_6H_6	benzene	liq	SEL	BP	353.22	0.13	EOS	2012THO
		sol	SEL1	MP	278.67	0.02	MP	1996LIN
		liq		BP	353.22	0.13	EOS-rev	2018LEM
				BP	353.2		BP comp	2016HUR
				BP	353.216	0.084	BP rev	2012KRO
				BP	353.3	0.2	VLE	1991DI
				BP	353.3	0.6	VP isoten	1971EON
				BP	353.2		VLE	1960KYL
				BP	353.25	0.15	BP rev	1947FEN
				BP	353.25	0.07	VP	1945WIL
				BP	353.4		BP rev	1935LES
		sol		MP	278.64	0.04	SLE	1986SNO
				MP	278.8	0.2	MP	1979MAH
				MP	278.6	0.1	MP	1970STO
C_7H_8	toluene	liq	SEL	BP	383.75	0.04	EOS	2006LEM
		sol	SEL1	MP	178.2	0.2	MP	1976RAD
				BP	383.75	0.04	EOS-rev	2018LEM
				BP	383.8		BP comp	2016HUR
				BP	383.8		VLE	1999TRE
				BP	383.8	0.2	VLE	1991DI
				BP	383.8		VLE	1991AIZ
				BP	383.80	0.15	BP rev	1947FEN
				BP	383.77	0.07	VP	1945WIL
				BP	383.7		BP rev	1935LES
C_8H_{10}	1,2-dimethylbenzene	liq	SEL	BP	417.56	0.07	VP	1945WIL
				BP	417.539	0.028	BP rev	2019DIK
				BP	417.52	0.19	EOS-rev	2018LEM
				BP	417.52	0.19	EOS	2012ZHO
				BP	417.40	0.15	VP extrap	1967AMB
				BP	417.9	0.2		1955TIM
				BP	417.55	0.15	BP rev	1947FEN
				BP	417.6		BP rev	1935LES
	1,3-dimethylbenzene	liq	SEL	BP	412.25	0.07	VP	1945WIL
				BP	412.23	0.06	BP rev	2019DIK
				BP	412.21	0.07	EOS-rev	2018LEM
				BP	412.21	0.07	EOS	2012ZHO

				BP	412.23	0.07	BP rev	2012KRO
				BP	412.2	0.2	VLE	1991DI
				BP	411.11	0.15	VP extrap	1967AMB
				BP	412.3	0.2	GLC	1957DES
				BP	412.30	0.15	BP rev	1947FEN
				BP	412.4		BP rev	1935LES
	1,4-dimethylbenzene	liq	SEL	BP	411.47	0.05	EOS	2012ZHO
				BP	411.47	0.07	EOS-rev	2018LEM
				BP	411.47	0.07	EOS	2012ZHO
				BP	411.467	0.064	BP rev	2012KRO
				BP	411.4	0.2	VLE	1990WIS
				BP	411.53	0.06	VP ebul	1974OSB
				BP	411.11	0.15	VP extrap	1967AMB
				BP	411.55	0.15	BP rev	1947FEN
				BP	411.50	0.07	VP	1945WIL
				BP	411.6		BP rev	1935LES
	ethylbenzene	liq	SEL	BP	408.96	0.15	VP	1967AMB
				BP	409.32	0.09	BP rev	2019DIK
				BP	409.31	0.11	EOS-rev	2018LEM
				BP	409.3		BP comp	2016HUR
				BP	409.31	0.11	EOS	2012ZHO
				BP	409.15	0.20	VLE	1991DI
				BP	409.40	0.15	BP rev	1947FEN
				BP	409.34	0.07	VP	1945WIL
				BP	409.3		BP rev	1935LES
C_9H_{12}	1,2,3-trimethylbenzene	liq	SEL	BP	449.23	0.15	VP	1967AMB
				BP	449.235	0.093	BP rev	2019DIK
				BP	449.1			1956FIE
				BP	449.3		BP	1954SCH
				BP	449.23	0.10	VP	1949FOR
				BP	449.2			1948REY
				BP	449.25	0.15	BP rev	1947FEN
	1,2,4-trimethylbenzene	liq	SEL	BP	442.50	0.15	VP	1967AMB
				BP	442.52	0.18	BP rev	2019DIK
				BP	442.5		VLE	1979KUR
				BP	442.50	0.10	VP	1949FOR
				BP	442.35	0.15	BP rev	1947FEN
	1,3,5-trimethylbenzene	liq	SEL	BP	437.87	0.15	VP	1967AMB

				BP	437.85	0.14	BP rev	2019DIK
				BP	437.9			1951CHI
				BP	437.87	0.10	VP	1949FOR
				BP	437.85	0.15	BP rev	1947FEN
				BP	437.9			1946BOO
				BP	437.8			1943LEC
				BP	437.9		VP	1940STU
				BP	437.8			1933MAI
				BP	437.8		BP rev	1921TIM
	2-ethyltoluene	liq	SEL	BP	438.25	0.15	VP	1949FOR
				BP	438.29	0.14	BP rev	2019DIK
				BP	438.1			1956FIE
				BP	438.1			1951KUT
				BP	438.30	0.15	BP rev	1947FEN
	3-ethyltoluene	liq	SEL	BP	434.46	0.10	VP	1949FOR
				BP	434.44	0.16	BP rev	2019DIK
				BP	434.55	0.15	BP rev	1947FEN
	4-ethyltoluene	liq	SEL	BP	435.14	0.10	VP	1949FOR
				BP	435.13	0.26	BP rev	2019DIK
				BP	435.10	0.15	BP rev	1947FEN
	isopropylbenzene	liq	SEL	BP	425.54	0.20	VLE	1989CEP
				BP	425.53	0.14	BP rev	2019DIK
				BP	425.6		BP comp	2016HUR
				BP	425.54	0.15	VP	1967AMB
				BP	425.55	0.15	BP rev	1947FEN
				BP	425.54	0.07	VP	1945WIL
	n-propylbenzene	liq	SEL	BP	432.37	0.15	VP	1967AMB
				BP	432.36	0.07	BP rev	2019DIK
				BP	433.1		VLE	1988PAU
				BP	432.4		VLE	1968KES
				BP	432.6			1950BRY
				BP	432.32	0.10	VP	1949FOR
				BP	432.40	0.15		1949FOE
				BP	432.40	0.15	BP rev	1947FEN
				BP	432.2		BP rev	1945SMI
$C_{10}H_{14}$	1,2-diethylbenzene	liq	SEL	BP	456.57	0.10	VP	1949FOR
				BP	456.57	0.14	BP rev	2019DIK
				BP	456.2			1952BER

			BP	456.5			1949BIR
			BP	454.35	0.15	BP rev	1947FEN
			BP	456.7			1946KAR
1,3-diethylbenzene	liq	SEL	BP	454.25	0.15	VP	1949FOR
			BP	454.24	0.17	BP rev	2019DIK
			BP	454.4		BP	1949BIR
			BP	454.40	0.15	BP rev	1947FEN
			BP	454.8			1946GIB
1,4-diethylbenzene	liq	SEL	BP	456.90	0.10	VP	1949FOR
			BP	456.89	0.17	BP rev	2019DIK
			BP	456.90	0.15	VP	1967AMB
			BP	456.9			1960MAI
			BP	456.6			1952BER
			BP	456.90	0.15	BP rev	1947FEN
			BP	457			1946KAR
2-isopropyltoluene	liq	SEL	BP	451.50	0.15	BP rev	1947FEN
			BP	451.4	1.0	BP rev	2019DIK
			BP	451.3	1.4	BP rev	2012KRO
			BP	451.45	0.05	VP ebul	1959MCD
			BP	451.3	0.3		1950BOO
3-isopropyltoluene	liq	SEL	BP	448.4	0.4		1949BIR
			BP	448.1	1.1	BP rev	2019DIK
			BP	448.2	0.4	BP rev	2012KRO
			BP	448.06	0.05	VP ebul	1959MCD
			BP	448.35	0.15	BP rev	1947FEN
4-isopropyltoluene	liq	SEL	BP	450.27	0.05	VP ebul	1959MCD
			BP	450.28	0.08	BP rev	2019DIK
			BP	450	4	BP rev	2012KRO
			BP	450.3			2010HAY
			BP	450.30	0.15	BP rev	1947FEN
Isobutylbenzene	liq	SEL	BP	445.95	0.15	BP rev	1947FEN
			BP	445.88	0.14	BP rev	2019DIK
n-butylbenzene	liq	SEL	BP	456.42	0.10	VP	1949FOR
			BP	456.42	0.08	BP rev	2019DIK
			BP	456.42	0.15	VP	1967AMB
			BP	456.5		BP	1949BIR
			BP	456.25	0.15	BP rev	1947FEN
sec-butylbenzene	liq	SEL	BP	446.30	0.15	BP rev	1947FEN

				BP	446.44	0.03	BP rev	2019DIK
	tert-butylbenzene	liq	SEL	BP	442.27	0.15	VP	1949FOR
				BP	442.26	0.03	BP rev	2019DIK
				BP	442.3		BP	1955RUS
				BP	442			1954CAD
				BP	442.30	0.15		1949FOE
				BP	442.6		BP	1949BIR
				BP	442.1			1947LEG
				BP	442.25	0.15	BP rev	1947FEN
				BP	442			1946RUE2
				BP	442.5		BP rev	1945SMI
				BP	442			1945GRE
Alkenylbenzenes								
C_8H_8	ethenylbenzene	liq	SEL	BP	418.5	0.3		1950BOO
				BP	418.5	0.4	BP rev	2019DIK
				BP	418.3		BP comp	2016HUR
				BP	418.4	0.9	BP rev	2012KRO
				BP	418.8	0.3	VLE	1955JUN
				BP	418.30	0.15	VP	1955DRE
Benzocycloalkanes								
C_9H_{10}	benzocyclopentane	liq	SEL	BP	450.9			2016CHI
				BP	450.96	0.11	BP rev	2019DIK
				BP	450.9		VP	1978OSB
				BP	451.0	0.2	BP rev	1947FEN
				BP	451.0		BP rev	1944BOO
$C_{10}H_{12}$	benzocyclohexane	liq	SEL	BP	480.6	0.5		1953KAR
				BP	480.3	0.5	BP rev	2019DIK
				BP	480.2		BP comp	2016HUR
				BP	480.3	0.4	BP rev	2012KRO
				BP	480.2			1955HAM
				BP	480.5	0.2	VP	1922HER
Benzocycloalkenes								
C_9H_8	benzocyclopentene	liq	SEL	BP	455.72	0.15	BP rev	1947FEN
				BP	455.72	0.23	BP rev	2019DIK
				BP	455.4		GLC	1967COO
				BP	454.7	0.5	VP rev	1947STU
Alkylnapthalenes								
$C_{10}H_8$	naphthalene	sol	SEL	MP	353.4	0.3	DSC	1980KRA

		liq	SEL1	BP	491.13	0.10	EOS	1993CHI
				BP	491.1	0.0	BP rev	2019DIK
				BP	491.1		BP comp	2016HUR
				BP	491.137	0.024	BP rev	2012KRO
				BP	491.5		VP ebul	1990AMB
				BP	491.7			1981WIL
				BP	490.73	0.15	VP	1968FOW
				BP	491.10	0.15	VP	1967AMB
				BP	491.11	0.10	VP	1955CAM
				BP	491.2	0.3		1943LEC
				BP	491.0	0.4	VP isoten	1923MOR
		sol		MP	353.3	0.5	VLE	1986SCH
				MP	353.43	0.02	rev	1984SZA
				MP	353.8	0.2	MP	1980RAD
$C_{11}H_{10}$	1-methylnaphthalene	liq	SEL	BP	517.84	0.10	VP	1955CAM
		sol	SEL1	MP	242.65	0.15	MP	1954HIP
		liq		BP	517.78	0.17	BP rev	2019DIK
				BP	517.9		BP comp	2016HUR
				BP	517.78	0.21	BP rev	2012KRO
				BP	518.0	0.5	GLC	1967COO
				BP	516.15	0.15	VP	1955MYE
		sol		MP	242.52	0.06	rev	1955STR
	2-methylnaphthalene	sol	SEL	MP	307.3	0.4	MP	1958RAM
		liq	SEL1	BP	514.25	0.15	VP	1981WIE
				BP	514.23	0.17	BP rev	2019DIK
				BP	514.2			2013NIK
				BP	514.24	0.21	BP rev	2012KRO
				BP	514.20	0.10	VP rev	1955CAM
				BP	514.3		VLE	1949OTH
				BP	514.3			1940MAI
		sol		MP	307.7	0.2	MP	1954HIP
Polycyclic Aromatics								
$C_{12}H_8$	acenaphthylene	sol	SEL	MP	366.4	1.0	MP	1965BOY
		liq	SEL1	BP	551	5	BP est	2019DIK
				BP	553.2		BP rev	2014HAY
	biphenylene	sol	SEL	MP	384.4	0.5	MP	1974YOK
		liq	SEL1	BP	548.5	3.0	BP est	2019DIK
$C_{12}H_{10}$	acenaphthene	sol	SEL	MP	364.0	1.0	MP	1990DON

		liq	SEL1	BP	550.4	0.4	VP isoten	1923MOR
				BP	550.6	0.3	BP rev	2019DIK
$C_{13}H_{10}$	fluorene	liq	SEL	BP	570.2	1.0	VP	1982SIV
		sol	SEL	MP	388	2	MP SLE	1989SED
		liq		BP	570.7	0.7	BP rev	2019DIK
				BP	569.6			1943LEC
				BP	570.2	0.4	VP isoten	1923MOR
$C_{14}H_{10}$	anthracene	sol	SEL	MP	489.5	0.3	MP	1988COO
		liq	SEL1	BP	614.9	0.4	VP isoten	1923MOR
				BP	614.093	0.011	BP rev	2019DIK
				BP	613.1			1931BUR
	phenanthrene	sol	SEL	MP	372.7	0.3	MP	1990DON
		liq	SEL1	BP	609.00	0.06	VP ebul	1975OSB
				BP	611.7	0.8	BP rev	2019DIK
				BP	605.3			1981WIL
				BP	611.5	0.4	VP isoten	1923MOR
		sol		MP	372.8	0.3	MP	1980RAM
$C_{16}H_{10}$	fluoranthene	sol	SEL	MP	381.0	0.3	MP	1973CAS
		liq	SEL1	BP	660	5	VP	1955TSY
				BP	647	6	BP est	2019DIK
	pyrene	sol	SEL	MP	424.3	0.6	MP	1987JUD
		liq	SEL1	BP	668	5	VP	1955TSY
				BP	662	4	BP est	2019DIK
$C_{18}H_{12}$	naphthacene	sol	SEL	MP	613	2	MP	1952INO
		liq	SEL1	BP	716	2	BP	1967WAK
				BP	714	5	BP est	2019DIK
$C_{20}H_{12}$	perylene	sol		MP	550.9	2.3	TP	2019DIK
$C_{24}H_{12}$	coronene	sol	SEL	MP	710.5	0.5	MP	1980SMI
		liq	SEL1	BP	798.2		BP rev	1989WEA

OXIDIZED HYDROCARBONS								
Carbon Oxides								
CO_2	carbon dioxide	sol	SEL	Sub	194.686	0.003	sub rev	1996BED
				Sub	194.685	0.003	EOS-rev	2018LEM
				Sub	194.685	0.003	EOS	1996SPA
				Sub	194.685	0.003	sub VP	1966BAR
				Sub	194.686	0.006	sub VP	1963LOV
				Sub	194.7	0.1	sub VP	1956AMB
				Sub	194.7	0.1	sub VP	1937GIA
				Sub	194.7	0.1	sub VP	1933MEY
CO	carbon monoxide	gas	SEL	BP	81.64	0.26	EOS	1979BRO
		sol	SEL1	TP	68.2		EOS	2006LEM
		gas		BP	81.6		EOS-rev	2018LEM
				BP	81.6		EOS	2006LEM
				BP	81.61	0.05	VP	1932CLA
		sol		TP	68.2		EOS-rev	2018LEM
Alkanols								
CH_4O	methanol	liq	SEL	BP	337.63	0.12	EOS	1993DER
				BP	337.63	0.12	EOS-rev	2018LEM
				BP	337.9		BP comp	2016HUR
				BP	337.63	0.16	BP rev	2012KRO
				BP	337.4		VLE	1998BLA
				BP	337.65	0.15	VLE	1998ARC
				BP	337.7		VLE	1997COM
				BP	337.5		VLE	1995RED
				BP	337.7		VLE	1992HIA
				BP	337.7		VLE	1991KAT
				BP	337.9		VLE	1991CAB
				BP	337.6		VLE	1990GUL
				BP	337.8		VLE	1988WIS
				BP	337.7		VLE	1978OCH
				BP	337.71	0.03	VLE	1973MAT
				BP	337.7		VLE	1970KIR
				BP	337.70	0.15	VP	1970AMB
				BP	337.4			1970AMB
C_2H_6O	ethanol	liq	SEL	BP	351.6	0.5	EOS	2014SCH
				BP	351.6	0.5	EOS-rev	2018LEM
				BP	351.4		BP comp	2016HUR

				BP	351.39	0.19	BP rev	2012KRO
				BP	351.44	0.10	VLE	1998ARC
				BP	351.5		VLE	1997COM
				BP	351.4		VLE	1995HIA
				BP	351.5		VLE	1991KAT
				BP	351.5		VLE	1985DRI
				BP	351.5		VLE	1979THO
				BP	351.45	0.15	VP	1970AMB
				BP	351.5		VLE	1960COP
				BP	351.45	0.15	VLE	1949KRE
C_3H_8O	1-propanol		liq	SEL	BP	370.3	0.2	VLE	1995HIA
					BP	370.11	0.23	BP rev	2019DIK
					BP	370.4		BP comp	2016HUR
					BP	370.19	0.15	BP rev	2012KRO
					BP	370.36	0.15	VLE	2010GAO
					BP	370.30	0.15	VP	1970AMB
					BP	370.35	0.15	VP	1969KEM
	isopropanol		liq	SEL	BP	355.39	0.08	VP	1963BID
					BP	355.39	0.18	BP rev	2019DIK
					BP	353.5		BP comp	2016HUR
					BP	356.36	0.13	BP rev	2012KRO
					BP	355.42	0.13	VLE	1995HIA
					BP	355.7		VLE	1990GUL
					BP	355.5		VLE	1985RAO2
					BP	355.6		VLE	1985DRI
					BP	355.0		VLE	1980YOS
					BP	355.5		VLE	1971NAG
					BP	355.5		VLE	1966KAT
					BP	355.42	0.15	VLE	1960TER
$C_4H_{10}O$	1-butanol		liq	SEL	BP	390.8	0.2	VLE	1996GON
					BP	390.6	0.3	BP rev	2019DIK
					BP	390.79	0.16	BP rev	2012KRO
					BP	390.8		VLE	1995WIS
					BP	390.7		VLE	1995RED
					BP	390.8		VLE	1992TAN
					BP	390.8		VLE	1991CAB
					BP	390.9		VP	1988GIE
					BP	390.9		VLE	1988AQU

			BP	390.8		VLE	1987KRI
			BP	390.8		VLE	1978TAM
			BP	390.9		VLE	1970KAT
			BP	391.02	0.15	VP	1969KEM
			BP	391.4	0.2	VLE	1965HES
			BP	390.88	0.12	VP	1963BID
	2-butanol	liq	SEL	BP	372.66	0.14	VP	1963BID
				BP	372.4	0.6	BP rev	2019DIK
				BP	372.56	0.18	BP rev	2012KRO
				BP	372.6		VLE	2011LLA
				BP	372.7		VLE	1998FEN
				BP	372.6		VLE	1987KRI
				BP	372.4		VLE	1985RAO
				BP	372.6			1960SKI
				BP	372.5		VLE	1953HEL
	isobutanol	liq	SEL	BP	380.90	0.15	VLE	1995RED
				BP	380.84	0.10	BP rev	2019DIK
				BP	380.98	0.03	BP rev	2012KRO
				BP	381.0		VLE	1988AQU
				BP	380.9		VLE	1987KRI
				BP	381.1		VLE	1981RAV
				BP	380.9		VLE	1975WIS
				BP	381.04	0.05	VP	1963BID
				BP	380.9			1962BRO
	tert-butanol	sol	SEL	MP	298.9	0.1	MP	1988KIM
		liq	SEL1	BP	355.50	0.15	VP	1963BID
				BP	355.51	0.06	BP rev	2019DIK
				BP	355.49	0.09	BP rev	2012KRO
				BP	355.6		VLE	1999LOR
				BP	355.3			1995RED
				BP	355.7		VLE	1988WIS3
				BP	355.6		VLE	1988AQU
				BP	355.6		VLE	1987KRI
				BP	355.5		VLE	1977GOV
				BP	355.47	0.15	VP	1969BRO
				BP	355.49	0.15	VP	1963BEY
				BP	355.4			1956STU
				BP	355.6			1956OMU

$C_5H_{12}O$	1-pentanol	liq	SEL	BP	410.9	0.3	VLE	1991YOS
				BP	411.0	0.9	BP rev	2019DIK
				BP	411.11	0.26	BP rev	2012KRO
				BP	411.1			1995RED
				BP	410.2		VLE	1988WIS
				BP	411			1982KAR
				BP	410.8		VLE	1976TAM
				BP	411.2			1974RAO
				BP	411.2		VLE	1972MIL
				BP	410.9			1970AMB
	2-methyl-1-butanol	liq	SEL	BP	402.14	0.17	VP ebul	2010CEN
				BP	402.01	0.22	BP rev	2019DIK
				BP	402.15	0.07	BP rev	2012KRO
				BP	401.8	0.5	VLE	1953MCK
				BP	403.8	0.2	VP	1935BUT
	2-methyl-2-butanol	liq	SEL	BP	375.30	0.17	VP ebul	2010CEN
				BP	375.22	0.26	BP rev	2019DIK
	2-pentanol	liq	SEL	BP	392.48	0.17	VP ebul	2010CEN
				BP	392.39	0.22	BP rev	2019DIK
				BP	392.25	0.17	VLE	2012MAR
				BP	392.22	0.17	VLE	2009GIE
				BP	393.02	0.25	VLE	1984RAO
				BP	392.33	0.17	VP ebul	1963THO
				BP	392.29	0.15	VP	1935BUT
	3-methyl-2-butanol	liq	SEL	BP	385.03	0.17	VP ebul	2010CEN
				BP	384.63	0.27	BP rev	2019DIK
				BP	385.6		VLE	1953MCK
				BP	384.6			1937GIN
				BP	386.1		VLE	1930LEC
				BP	386.6			1916WIL
	3-pentanol	liq	SEL	BP	388.62	0.17	VP ebul	2010CEN
				BP	388.57	0.24	BP rev	2019DIK
	isopentanol	liq	SEL	BP	404.73	0.17	VP ebul	2010CEN
				BP	404.57	0.27	BP rev	2019DIK
				BP	405.2		BP comp	2016HUR
				BP	403.95	0.13	BP rev	2012KRO
				BP	404.55	0.06	VLE	2010CEP
				BP	403.5		VLE	1992TAN

				BP	403.9		VP	1986MAR
				BP	403.8		VLE	1985RAO
				BP	404.9		VLE	1981RAV
				BP	405.2		VLE	1972MIL
				BP	405.2		VLE	1965RED
				BP	405		VLE	1960TER
Glycols								
$C_2H_6O_2$	1,2-ethanediol	liq	SEL	BP	470.3	0.2	EOS-rev	2018LEM
				BP	470.5	0.9	BP rev	2019DIK
				BP	470.35	0.04	VLE	2013QIA
				BP	470.3	0.3	VLE	2013PLA
				BP	470.36	0.10	VP	2012KAM
				BP	470.4	0.4	VLE	2004NAG
				BP	470.5	0.5	VLE	1982DIZ
				BP	470.50	0.03	VP	1981MAR
				BP	470.44	0.06	VP	1981AMB
				BP	470.4	0.5	VLE	1971SOK
				BP	470.38	0.25	VLE	1959KOG
				BP	470.73	0.25	VP rev	1952JON
				BP	470.4	0.5	VLE	1949OTH
				BP	471.0	0.5	BP rev	1935TIM
				BP	470.4	0.5	BP	1931SMY
$C_3H_8O_2$	1,2-propanediol	liq	SEL	BP	461.2	0.8	EOS	2021EIS
				BP	461.5	0.4	BP rev	2019DIK
				BP	461.2		VLE	2013ZHA
				BP	461.31	0.03	VLE	2011MAT
				BP	460.43	0.23	EOS	2002STE
				BP	461.2	0.4	VP comp	1999DEA
				BP	461.0	0.4	VP	1955TIM
				BP	461.4	0.4	VP comp	1954MAR
				BP	459.8	1.0	VP	1952WES
				BP	459.2	1.5	VP	1950CLE
				BP	460.6	0.6	VP	1935SCH
	2-methoxyethanol	liq	SEL	BP	397.54	0.15	VLE	2012RED
				BP	397.47	0.04	BP rev	2019DIK
				BP	397.41	0.07	BP rev	2012KRO
				BP	397.6		VP	2012BEJ
				BP	397.4		VLE	2010MAR

				BP	397.5	0.4	VLE	1995RED
				BP	397.6	0.4	VLE	1995KRI
				BP	397.7		VLE	1979CHA
				BP	397.4			1970QUI
				BP	397.29	0.15	VP	1956PIC
Sugars								
$C_3H_8O_3$	glycerin	liq	SEL	BP	563.0	1.3	BP	2019DIK
		sol	SEL1	MP	291.1	0.5	MP	1958COS
$C_6H_{10}O_5$	cellulose	sol	SEL	MP	408.2		MP	2020POD
$C_6H_{12}O_6$	alpha-D-glucose	sol	SEL	MP	421.8	0.6	MP	2004HUR
		gas	SEL1	BP	706	50	est	2019DIK
		sol		MP	414		MP	1996DOM
				MP	423.2		MP	1983RAE
	fructose	sol	SEL	MP	376.7	0.3	MP	2004HUR
				MP	378.2		MP	1995FAN
$C_{12}H_{22}O_{11}$	sucrose	sol	SEL	MP	456	4	MP	2004HUR
				MP	459	3	dec	2021EPA
				MP	461.2		MP	2001GLO
				MP	458.2		MP	1983RAE
				MP	462	3	MP	1950KOF
Phenols								
C_7H_8O	2-methylphenol	liq		BP	464.1		VP	1958BID
		sol	SEL	MP	304.14	0.10	MP	1960AND
		liq	SEL1	BP	464.14	0.10	VP rev	1949DRE2
				BP	464.15	0.05	BP rev	2019DIK
				BP	464.3			1947LEC
				BP	464.30	0.18	VP	1947GOL
				BP	463.9			1944PAR
		sol		MP	464.1	0.3	MP	1949DRE
	4-methylphenol	sol	SEL	MP	307.84	0.20	MP	1960AND
		liq	SEL1	BP	474.99	0.10	VP rev	1949DRE2
				BP	475.10	0.28	BP rev	2019DIK
				BP	475		VLE	1968TAY
				BP	474.90	0.18	VP	1947GOL
Alkyl ethers								
C_2H_6O	dimethyl ether	gas	SEL	BP	248.37	0.09	EOS	2011WU
				BP	248.37	0.09	EOS-rev	2018LEM
				BP	248.34	0.15	VP	1941KEN

C_3H_8O	ethyl methyl ether	gas	SEL	BP	279.7	0.5		1941IPA
				BP	280.59	0.19		2019DIK
				BP	280.7		VP rev	1947STU
				BP	281.2			1924BER
$C_4H_{10}O$	diethyl ether	liq	SEL	BP	307.56	0.15	VP	1972AMB
				BP	307.59	0.03	BP rev	2019DIK
				BP	307.7		VLE	2011GAO
				BP	307.63	0.15	VP	1922TAY
	isopropyl methyl ether	liq	SEL	BP	303.90	0.02		1976AMB
				BP	303.917	0.014		2019DIK
	n-propyl methyl ether	liq	SEL	BP	311.8			1976AMB
				BP	311.70	0.03		2019DIK
				BP	312.2		VP rev	1947STU
$C_5H_{12}O$	*n*-butyl methyl ether	liq	SEL	BP	343.29	0.02	VLE	2007BOU
				BP	343.3	0.0		2019DIK
				BP	343.3			1976AMB
	tert-butyl methyl ether	liq	SEL	BP	328.20	0.15	VLE	1999MON
				BP	328.23	0.13	BP rev	2019DIK
$C_6H_{14}O$	diisopropyl ether	liq	SEL	BP	341.6	0.3	VLE	1996RES
				BP	341.58	0.14	BP rev	2019DIK
				BP	341.4	0.3	VLE	1999MON
				BP	341.49	0.15	VP	1969CID
	di-*n*-propyl ether	liq	SEL	BP	363.25	0.04	VP	1973MEY
				BP	363.22	0.03	BP rev	2019DIK
				BP	364.2		VLE	1972MAR
				BP	359.50	0.15	VP	1969CID
				BP	363.9			1950SPU
	isobutyl ethyl ether	liq	SEL	BP	354.2	1.0		1932NOR
				BP	354.2	1.9		2019DIK
Aldehydes								
CH_2O	formaldehyde	gas	SEL	BP	254.1	0.2	VP	1935SPE
				BP	254.0	0.4	BP rev	2019DIK
				BP	253.9		BP comp	2016HUR
				BP	253.4	0.6	BP rev	2012KRO
				BP	254.05	0.15	BP rev	1977REI
C_2H_4O	acetaldehyde	gas	SEL	BP	293.56	0.15	VLE	1950COL
				BP	293.8	0.5	BP rev	2019DIK
				BP	294.2		BP comp	2016HUR

				BP	293.6	0.8	BP rev	2012KRO
				BP	293.5	0.3	VLE	1963BUL
				BP	293.9	0.3		1955SHI
				BP	293.9	0.6		1950CHR
C_3H_6O	propanal	liq	SEL	BP	321.19	0.15	VLE	2010GAO
				BP	321.15	0.08	BP rev	2019DIK
				BP	321.12	0.03	VLE	1984ENG
				BP	321.17	0.05		1977SVO
				BP	321.17	0.03	VLE	1977BOU
				BP	321.19	0.03	VLE	1973MAT
				BP	321.20	0.03		1972COU
				BP	321.15	0.03	VLE	1953MCK
				BP	321.1			1962TJE
C_4H_8O	butanal	liq	SEL	BP	348.0	0.4	VLE	1985HSU
				BP	347.95	0.15	BP rev	2019DIK
				BP	348.3	0.5	BP rev	2012KRO
				BP	347.9	0.3	VLE	1984ENG
				BP	348.33	0.25	VP	1959SEP
				BP	347.4	0.5		1955BRO
				BP	347.7	0.5	VLE	1953MCK
				BP	348.4	0.5		1943HUR
				BP	348.0	0.3		1938DOL
				BP	347.8	0.5		1938COO
				BP	348.9	0.5		1922TIM
	isobutanal	liq	SEL	BP	337.3	0.5		1941HEA
				BP	337.19	0.11	BP rev	2019DIK
				BP	337.25	0.14	BP rev	2012KRO
				BP	337.26	0.25	VP	1959SEP
Alkenals								
C_3H_4O	1-propenal	gas	SEL	BP	264		BP est	2021CHE
	2-propenal	liq	SEL	BP	325.4	0.3		1979MAR
				BP	325.46	0.10	BP rev	2019DIK
				BP	325.7		BP comp	2016HUR
				BP	325.48	0.11	BP rev	2012KRO
				BP	325.71	0.18	VP rev	1947STU
Ketones								
C_3H_6O	acetone	liq	SEL	BP	329.22	0.29	EOS	2006LEM
				BP	329.22	0.29	EOS-rev	2018LEM

				BP	329.2	0.2	VLE	1999TRE
				BP	329.5		VLE	1990GUL
				BP	329.2		VP	1986TAK
				BP	329.42	0.15	VP	1974AMB
				BP	329.0		VLE	1970WIL
				BP	329.5			1955KOC
C_4H_8O	butanone	liq	SEL	BP	352.74	0.03	VLE	1973MAT
				BP	352.71	0.02	BP rev	2019DIK
				BP	352.7		VLE	2011LLA
				BP	352.7		VLE	2002DEL
				BP	352.8		VLE	1994YAH
				BP	352.63	0.15	VP	1961NIC
$C_5H_{10}O$	2-pentanone	liq	SEL	BP	375.45	0.15	VLE	1973SCH
				BP	375.38	0.05		2019DIK
				BP	375.1			2003AUC
				BP	375.3		VP	1975AMB
				BP	376.0			1966MEY
	3-pentanone	liq	SEL	BP	375.11	0.06	VP	1965COL
				BP	375.08	0.06	BP rev	2019DIK
				BP	376.41	0.10	VP rev	1949DRE2
Carboxylic Acids								
CH_2O_2	formic acid	liq	SEL	BP	374.1	0.4	VLE	2011BAS
		sol	SEL1	MP	281.5	0.2	MP	1981KOH
		liq		BP	374.35	0.24	BP rev	2019DIK
				BP	374.4		VLE	2007INC
				BP	373.7		VLE	1990KAT
				BP	374.8		VP	1987AMB2
				BP	373.6			1973LAK
				BP	373.8		VLE	1960CON
				BP	373.7			1952WAR
				BP	373.9		VP rev	1949DRE2
				BP	374.0		VLE	1949ALP
$C_2H_4O_2$	acetic acid	liq	SEL	BP	391.20	0.15	VLE	1991SAY
		sol	SEL1	MP	289.5	0.1	rev	1959MCD
		liq		BP	390.97	0.05	BP rev	2019DIK
				BP	391.1		VLE rev	1990HUI2
				BP	391.1		VLE	1988KAT
				BP	391.3		VLE	1968BAR

				BP	391.01	0.05	VP ebul	1959MCD
$C_3H_6O_2$	propanoic acid	liq	SEL	BP	414.0	0.3	VLE	1982WIS
				BP	414.04	0.10	BP rev	2019DIK
				BP	413.99	0.15	VLE	2010GAO
				BP	414.24	0.10	VP rev	1949DRE2
$C_4H_8O_2$	*n*-butanoic acid	liq	SEL	BP	436.42	0.10	VP rev	1949DRE2
				BP	436.4	0.4	BP rev	2019DIK
				BP	436.7		VLE	1976RAD
				BP	437.2		VLE	1954PUR
$C_5H_{10}O_2$	*n*-pentanoic acid	liq	SEL	BP	459.1	0.3		1964ADR
				BP	458.5	0.6		2019DIK
				BP	459.2			2012GUN
				BP	459.0		VP	1987AMB2
				BP	459.4			1955HAN2
				BP	459.0			1955GEN
$C_6H_{12}O_2$	*n*-hexanoic acid	liq	SEL	BP	478.2	0.5		1949PAT
				BP	477.7	0.8		2019DIK
				BP	477.3			1958BAK
				BP	478.2	-		1952JAM
				BP	478.2	-		1938VAN
				BP	478.1	-		1933KOH
Alkyl Esters								
$C_2H_4O_2$	methyl formate	liq	SEL	BP	305.1	0.3	VP	1928NEL
				BP	304.76	0.08	BP rev	2019DIK
$C_3H_6O_2$	ethyl formate	liq	SEL	BP	327.29	0.05	VLE	1998SOT
				BP	327.23	0.04	BP eval	2019DIK
	methyl acetate	liq	SEL	BP	330.11	0.15	VLE	2016MAT
				BP	330.2		VLE	2019JIA
				BP	329.81	0.06		2019DIK
				BP	330.1		VLE	2018SHA
				BP	330.0		VLE	1969HUD
$C_4H_8O_2$	ethyl acetate	liq	SEL	BP	350.21	0.15	VP	1965POL
				BP	350.15	0.05	BP rev	2019DIK
	methyl propanoate	liq	SEL	BP	352.75	0.25		2014RIO
				BP	352.40	0.15		2019DIK
				BP	351.7		VLE	1989SUS
				BP	352.85	0.25		1977SVO
				BP	352.9	-		1959TIM

$C_5H_{10}O_2$	methyl butanoate	liq	SEL	BP	375.74	0.25	VLE	2012RIO
				BP	375.36	0.12		2019DIK
				BP	375.8			2012AGA
				BP	375.0		VLE	2004ORT
				BP	375.5		VLE	2003ORT
				BP	373.7	-		1956SUM
				BP	375.8	-		1927LEC
				BP	375.9	-		1910YOU
	n-propylacetate	liq	SEL	BP	374.7	0.4		1977SVO
				BP	374.28	0.07		2019DIK
				BP	374.3			2015SUS
				BP	374.3		VLE	2013FER
				BP	374.6	-	VP	1965POL
				BP	374.9	-		1959TIM
Alkenyl Esters								
$C_4H_6O_2$	vinyl acetate	liq	SEL	BP	345.3	0.4	VLE	1965SWA
				BP	345.73	0.09	BP rev	2019DIK
				BP	345.88	0.15	VLE	1963CAP
$C_5H_8O_2$	ethyl propenoate	liq	SEL	BP	372.59	0.15	VLE	2013LOM
				BP	372.0	0.5	BP rev	2019DIK
				BP	370.2		VP rev	1987DAU
				BP	372.6		VLE	1973FIL
				BP	372.69	0.15	VP rev	1947STU
	methyl 2-methylpropenoate	liq	SEL	BP	369.7	0.5	VP	1956BRO
				BP	373.76	0.12	BP rev	2019DIK
Alkanoic Anhydrides								
$C_4H_6O_3$	acetic anhydride	liq	SEL	BP	412.62	0.15		1976RAD
				BP	412.65	0.05		2019DIK
				BP	412.4		VP	1987AMB
				BP	411.8		VP	1959MCD
				BP	412.5		VLE	1950NEL
$C_6H_{10}O_3$	propanoic anhydride	liq	SEL	BP	440.3	1.5		1961WRI
				BP	440.8	0.8		2019DIK
				BP	438.2			1958LEV
$C_8H_{14}O_3$	butanoic anhydride	liq	SEL	BP	471.4	2.0		1921TIM2
				BP	471.2	2.5		2019DIK
				BP	471.4			1961WRI
				BP	471.4		BP comp	1958LEV

Oxacycloalkanes								
C_2H_4O	oxacyclopropane	gas	SEL	BP	283.66	0.13	EOS	2015THO
				BP	283.59	0.04	BP rev	2019DIK
				BP	283.66	0.13	EOS-rev	2018LEM
				BP	283.59	0.05	VP ebul	1959MCD
				BP	283.65	0.15	VLE	1950COL
C_3H_6O	methyloxacyclopropane	liq	SEL	BP	307.56	0.25	VLE	1985KOL
				BP	307.34	0.07		2019DIK
				BP	307.27	0.14	EOS-rev	2018LEM
				BP	307.4		VLE	1989MUH
				BP	307.2		VP	1966BOT
				BP	307.9	-		1956PRI
				BP	308.2	-		1937MOU
				BP	308.0	-		1934ALL
	oxacyclobutane	liq	SEL	BP	320.73	0.10	VP	1980OSB
				BP	320.73	0.02		2019DIK
				BP	321.6			1960CHA
				BP	320.8			1934ALL
C_4H_8O	oxacyclopentane	liq	SEL	BP	339.15	0.15	VLE	1998WIS
				BP	339.14	0.06		2019DIK
				BP	339.1	-		1996KRI
				BP	338.9	-	VLE	1975SAD
				BP	339.1	-		1946BOO
$C_5H_{10}O$	oxacyclohexane	liq	SEL	BP	361.36	0.20	VLE	2012MEJ
				BP	361.32	0.14		2019DIK
				BP	361.2	-		2005GIN
				BP	361.2	-	VLE	2000ROD
				BP	361.1	-		1964MOE
				BP	361.2	-		1957KIR
				BP	361.2	-		1934ALL
Oxacycloalkadienes								
C_4H_4O	oxacyclopentadiene	liq	SEL	BP	304.51	0.08	VP	1952GUT2
				BP	304.50	0.07	BP rev	2019DIK
C_5H_6O	2-methyloxacyclopentadiene	liq	SEL	BP	338.4	0.5	VP isoten	1971EON
				BP	337.1	0.4	BP rev	2019DIK
Oxacycloketones								
C_3H_4O	cyclopropanone	liq	SEL	BP	333	18	BP est	2019DIK
C_4H_6O	cyclobutanone	liq	SEL	BP	372.9	0.5		1972WOL

				BP	371.95	0.04	BP rev	2019DIK
				BP	372.9	0.5	BP	1972WOL
				BP	372.2			1949ROB
				BP	367.8	0.2	VP	1942BEN
C_5H_8O	cyclopentanone	liq	SEL	BP	403.9	0.3	BP	1972WOL
				BP	403.68	0.07	BP rev	2019DIK
				BP	403.8		BP	1937TIM
$C_6H_{10}O$	cyclohexanone	liq	SEL	BP	428.57	0.04	VP	1973MEY
				BP	428.54	0.10	BP rev	2019DIK
				BP	428.6	0.3	BP	1965GRO
$C_7H_{12}O$	2-methylcyclohexanone	liq	SEL	BP	438.0	0.5	VLE	1993BUR
				BP	437.56	0.05	BP rev	2019DIK
				BP	438.2	0.5	BP	1940WHI
	3-methylcyclohexanone	liq	SEL	BP	442.7	0.5	BP	1940WHI
				BP	442.41	0.25	BP rev	2019DIK
	4-methylcyclohexanone	liq	SEL	BP	444.6	0.5	BP	1940WHI
				BP	444.1	0.3	BP	2019DIK
Dioxanes and Trioxanes								
$C_3H_6O_3$	1,3,5-trioxane	sol	SEL	MP	335.7	2.0	MP	1963LEV
		liq	SEL1	BP	387.2	0.4	VLE	1966SER
		sol		MP	333.4	2.0	TP	1988VAN
$C_4H_8O_2$	1,3-dioxane	liq	SEL	BP	378.1	0.5	BP	1967PIH
				BP	377.9	2.8	BP est	2019DIK
				BP	377.6	0.5	BP	1972RAK
	1,4-dioxane	liq	SEL	BP	374.3	0.3	VLE	1956MCC
				BP	374.4	0.4	BP rev	2019DIK
				BP	374.44	0.15	VP	1938CRE
Furandione and D-Camphor								
$C_{10}H_{16}O$	D-camphor	sol	SEL	MP	452	10	MP	1992AND
				MP	463.4		MP	1990DON
				MP	452.0		MP	1979MJO
$C_4H_2O_3$	2,5-furandione	sol	SEL	MP	325.3	0.5	MP	1983DEW
		liq	SEL1	BP	478	5	VP rev	1947STU
				BP	476	11	BP est	2019DIK
				BP	473	5	VLE	2002GU
				BP	473	5	VP rev	1947ALD
Aromatic Alcohols								
C_6H_6O	phenol	sol	SEL	MP	314.05	0.15	MP	1960AND

		liq	SEL1	BP	454.91	0.10	VP rev	1949DRE2
				BP	454.96	0.17	BP rev	2019DIK
				BP	455.19	0.18	VP	1947GOL
C_7H_8O	3-methylphenol	liq	SEL	BP	475.50	0.20	VLE	1989CEP2
		sol	SEL1	MP	285.37	0.20	MP	1960AND
		liq		BP	475.4		BP rev	2019DIK
				BP	475.28	0.18	VP	1947GOL
				BP	475.9		BP rev	1937TIM
				BP	475.3		VLE	1921KEN
		sol		MP	285.1		MP	1937TIM
	benzyl alcohol	liq	SEL	BP	478.5	0.3	VLE	1998SEN
				BP	478.3	0.9	BP rev	2019DIK
				BP	478.6		VLE	1994RES
				BP	478.49	0.07	VP	1990AMB2
				BP	478.2	0.3	GLC	1977KUC
				BP	477.9			1967MAR
				BP	478.45	0.10	VP rev	1949DRE2
				BP	478.4		VLE	1947LEC2
				BP	478.9		BP rev	1922TIM
Aromatic Aldehydes and Acids								
C_7H_6O	benzaldehyde	liq	SEL	BP	451.15	0.20	VLE	1981RAO
				BP	452.4		VLE	1958LEV
				BP	451.68	0.18	VP rev	1947STU
				BP	452.4		VLE	1943LEC
				BP	452.2		VLE	1941EWE2
$C_7H_6O_2$	benzoic acid	sol	SEL	MP	395.50	0.04	MP	1989HAL
		liq	SEL1	BP	523.5	0.5	VP rev	1947STU
				BP	523.2	0.8	BP rev	2019DIK
				BP	522.2		BP rev	1989WEA
				BP	523.6			1931BUR
				BP	523.3			1930MAR
				BP	522.6		VP	1927KLO

NITROGEN-SUBSTITUTED HYDROCARBONS								
Hydrogen Cyanides								
CHN	hydrogen cyanide	liq	SEL	BP	298.8	0.3	VP	1926SIN
				BP	298.78	0.04	BP rev	2019DIK
Alkylamines								
CH_5N	methylamine	gas	SEL	BP	266.84	0.15	VP	1937AST
				BP	266.76	0.19	BP rev	2019DIK
C_2H_7N	ethylamine	gas	SEL	BP	289.79	0.18	VP rev	1947STU
				BP	289.80	0.09	BP rev	2019DIK
C_3H_9N	*n*-propylamine	liq	SEL	BP	320.38	0.06	VP ebul	1968OSB
				BP	320.36	0.05	BP rev	2019DIK
				BP	321.7	0.5	VP rev	1947STU
	isopropylamine	liq	SEL	BP	304.92	0.06	VP ebul	1968OSB
				BP	304.91	0.04	BP rev	2019DIK
$C_4H_{11}N$	isobutylamine	liq	SEL	BP	341.1	0.2		1977RAD
				BP	340.69	0.05		2019DIK
				BP	340.7		VP	1980OSB
				BP	340.9		VP	1979MAJ
				BP	341.1			1962HOL
				BP	340.9	-		1959COS
				BP	340.1			1951BAR
				BP	341.1			1949SCH
				BP	340.8		VP	1935SIM
				BP	341.2	-		1921TIM2
	n-butylamine	liq	SEL	BP	350.1	0.3	VLE	1971LET
				BP	350.17	0.13	BP rev	2019DIK
	tert-butylamine	liq	SEL	BP	317.19	0.06	VP ebul	1968OSB
				BP	317.18	0.04	BP rev	2019DIK
C_2H_7N	dimethylamine	gas	SEL	BP	280.02	0.15	VP	1939AST
				BP	280.3	0.4	BP rev	2019DIK
C_3H_9N	methylethylamine	liq	SEL	BP	305.6	0.5	VLE	1985WOL
				BP	305.8	0.6	BP rev	2019DIK
$C_4H_{11}N$	diethylamine	liq	SEL	BP	328.48	0.15		1971LET
				BP	328.48	0.13		2019DIK
				BP	328.6	-	VLE	1967NAK
				BP	328.5	-	VLE	1967HUM
				BP	328.5	-		1959COS
C_3H_9N	trimethylamine	gas	SEL	BP	276.00	0.15	VP	1944AST

				BP	276.07	0.24	BP rev	2019DIK
$C_6H_{15}N$	triethylamine	liq	SEL	BP	361.93	0.25	VLE	1962BIT
				BP	362.2	0.3	BP rev	2019DIK
Cycloalkylamines								
$C_6H_{13}N$	cyclohexylamine	liq	SEL	BP	406.98	0.15	VLE	1960NOV
				BP	406.8	0.3	BP rev	2019DIK
				BP	407.4			1940WHI
				BP	407.0			1939LEW
Azacycloalkanes								
C_2H_5N	azacyclopropane	liq	SEL	BP	328.6	1.0		1956SEA
				BP	327.4	0.5		2019DIK
C_3H_7N	azacyclobutane	liq	SEL	BP	333.5	1.5		2019DIK
				BP	336			1982BUC
C_4H_9N	azacyclopentane	liq	SEL	BP	359.71	0.15	VP	1959MCC
				BP	359.71	0.07	BP rev	2019DIK
$C_5H_{11}N$	azacyclohexane	liq	SEL	BP	379.37	0.06	VP ebul	1968OSB
				BP	379.34	0.13	BP rev	2019DIK
Methenamines								
$C_6H_{12}N_4$	methenamine	sol	SEL	MP	359	10	sub	2002VER
Azacycloalkadienes								
C_4H_5N	azacyclopentadiene	liq	SEL	BP	402.93	0.06	VP ebul	1968OSB
				BP	402.90	0.05	BP rev	2019DIK
				BP	399.5	0.6	VP isoten	1971EON
C_5H_7N	1-methylazacyclopentadiene	liq	SEL	BP	385.90	0.06	VP ebul	1968OSB
				BP	385.87	0.04	BP rev	2019DIK
				BP	384.7	0.6	VP isoten	1971EON
Alkanenitriles								
C_2H_3N	ethanenitrile	liq	SEL	BP	355.05	0.15	VP	1974DOJ
				BP	354.74	0.03	BP rev	2019DIK
C_3H_5N	propanenitrile	liq	SEL	BP	370.7	0.3	VP rev	1949DRE2
				BP	370.41	0.29	BP rev	2019DIK
C_4H_7N	butanenitrile	liq	SEL	BP	390.77	0.04	VP	1973MEY
				BP	390.74	0.04	BP rev	2019DIK
C_5H_9N	pentanenitrile	liq	SEL	BP	414.42	0.10	VP rev	1949DRE2
				BP	414.39	0.17	BP rev	2019DIK
$C_6H_{11}N$	hexanenitrile	liq	SEL	BP	436.61	0.04	VP	1973MEY
				BP	436.59	0.05	BP rev	2019DIK
				BP	436.3			1961WRI

				BP	436.88	0.10	VP rev	1949DRE2
Alkenenitriles								
C_3H_3N	propenenitrile	liq	SEL	BP	351.1	0.5	VLE	1964SEV
				BP	350.7	0.9	BP rev	2019DIK
Cyanogens								
C_2N_2	cyanogen	gas	SEL	BP	251.92	0.20	VP	1939RUE
				BP	251.954	0.002	BP rev	2019DIK
				BP	252.0		BP rev	1985MAJ
				BP	252.18	0.18	VP rev	1947STU
				BP	251.8		VP	1925PER
Alkylhydrazines								
$C_2H_8N_2$	1,1-dimethylhydrazine	liq	SEL	BP	335.4	0.3	VLE	1992FER
				BP	335.2	0.7	BP rev	2019DIK
				BP	337.1		BP rev	1989WEA
				BP	336.2		VP	1985MAJ
				BP	334.3		VP	1970KOB
				BP	335.3		VLE	1956CAR
				BP	335.57	0.20	VP	1953AST
Melamines								
$C_3H_6N_6$	melamine	sol	SEL	MP	627		MP	2005LID
Pyridines								
C_5H_5N	pyridine	liq	SEL	BP	388.36	0.06	BP rev	2019DIK
				BP	388.46	0.10		
				BP	388.36	0.06		
C_6H_7N	2-methylpyridine	liq	SEL	BP	402.52	0.08	VP	1963SCO
				BP	402.53	0.04	BP rev	2019DIK
Anilines								
	aniline	liq	SEL	BP	457.1	0.2	VLE	1979KUR
				BP	457.2	0.5	BP rev	2019DIK
				BP	457.7		VLE	1992GUP
				BP	457.0		VLE	1965DES
				BP	457.6			1962STE
				BP	457.1		VLE	1962STA
				BP	456.99	0.05		1962HAT
				BP	457.3	0.3	VLE	1959ELL
				BP	457.5		VLE	1950KOR
				BP	457.1			1949DRE
				BP	457.6		BP rev	1926TIM

$C_8H_{11}N$	*N*,*N*-dimethylaniline	liq	SEL	BP	466.5	0.4	BP	1976RAD
		sol	SEL1	MP	275.7	0.3	MP	1976RAD
		liq		BP	466.7	1.0	BP rev	2019DIK
				BP	466.5	0.5	VP rev	1947STU
				BP	466.5	0.4	BP	1946LEC
				BP	466.6	0.5	VP	1925NEL
Oxidized Amines								
CH_4N_2O	urea	sol	SEL	MP	406.2	0.5	TP	1972ZOR
				MP	405.6	0.4	TP	2019DIK
				MP	406.5	0.5	TP	2011RAI
				MP	405.8	0.5	TP	2010ZEN
				MP	406.5	0.5	TP	1987DEL
$C_6H_{15}NO_3$	triethanolamine	liq	SEL	BP	608	5	VP extrap	1959MCD
		sol	SEL1	MP	294.7	0.5	MP	1959MCD
		liq		BP	605	8	BP rev	2019DIK
				BP	623.2		BP rev	2014HAY
				BP	608.6		BP rev	2013ONE
Alkyl Nitrates and Nitroalkanes								
CH_3NO_3	methyl nitrate	liq	SEL	BP	338.0		VLE	1947LEC
				BP	338	3	BP rev	2019DIK
$C_3H_5N_3O_9$	nitroglycerin	sol	SEL	MP	286.7		MP	2001ONE
CN_4O_8	tetranitromethane	liq	SEL	BP	397.9		VP	1952EDW
		sol	SEL1	MP	287.1	0.5	MP	1955TIM
		liq		BP	399.2		BP rev	1985MAJ
CHN_3O_6	trinitromethane	sol	SEL	MP	292	3	MP	1939LEW
CH_3NO_2	nitromethane	liq	SEL	BP	374.34	0.08	VP	1954MCC
				BP	374.32	0.09	BP rev	2019DIK
Isocyanates								
$C_9H_6N_2O_2$	2,4-diisocyanatotoluene	liq	SEL	BP	524.8	2.0	VP	1975FRE
		sol	SEL1	MP	293.7	1.0	MP	2020FIS
		liq		BP	524		BP rev	2010HAY
				BP	529		VP	1990DAU
Nitro Aromatics								
$C_6H_5NO_2$	nitrobenzene	liq	SEL	BP	483.81	0.15	VLE	1952BRO
		sol	SEL1	MP	278.89	0.20	MP	1954WIT
		liq		BP	483.82	0.29	BP rev	2019DIK
		sol		MP	279.2	1.0	MP	1965MAL
$C_7H_5N_3O_6$	trinitrotoluene	sol	SEL	MP	355.1	1.0	MP	1990HUI

SULFUR-SUBSTITUTED HYDROCARBONS								
Alkanethiols								
CH_4S	methanethiol	gas	SEL	BP	279.05	0.10		1960MOR
				BP	279.10	0.06	BP rev	2019DIK
				BP	279.10	0.06	BP rev	2012KRO
				BP	279.05	0.15	BP ebul	1960HAI
				BP	279.10	0.15	VP ebul	1942RUS
C_2H_6S	ethanethiol	liq	SEL	BP	308.15	0.15	VP ebul	1966OSB
				BP	308.14	0.15	BP rev	2019DIK
				BP	308.14	0.15	BP rev	2012KRO
				BP	308.19	0.15		1953BIR
				BP	308.19	0.15	VLE	1949DEN
C_3H_8S	1-propanethiol	liq	SEL	BP	340.87	0.15	VP	1956PEN
				BP	340.84	0.15	BP rev	2019DIK
				BP	340.95	0.15	BP ebul	1960HAI
				BP	340.97	0.15	VLE	1949DEN
	isopropanethiol	liq	SEL	BP	325.71	0.15	VP ebul	1966OSB
				BP	325.69	0.15	BP rev	2019DIK
				BP	325.80	0.15	BP ebul	1956HAI
$C_4H_{10}S$	1-butanethiol	liq	SEL	BP	371.56	0.15	VP ebul	1966OSB
				BP	371.59	0.15	BP rev	2019DIK
				BP	371.20	0.15	BP ebul	1956HAI
	1-isobutanethiol	liq	SEL	BP	361.64	0.15	VP ebul	1966OSB
				BP	361.63	0.15	BP rev	2019DIK
				BP	361.65	0.15	BP ebul	1960HAI
	2-butanethiol	liq	SEL	BP	358.13	0.15	VP ebul	1966OSB
				BP	358.12	0.15	BP rev	2019DIK
				BP	358.20	0.15	BP ebul	1956HAI
$C_5H_{12}S$	1,1-dimethyl-1-propanethiol	liq		BP	372.35	0.15	BP ebul	1960HAI
			SEL	BP	372.28	0.15	VP ebul	1966OSB
				BP	372.28	0.15	BP rev	2019DIK
	1-pentanethiol	liq	SEL	BP	399.79	0.15	VP ebul	1966OSB
				BP	399.77	0.15	BP rev	2019DIK
	isopentanethiol	liq	SEL	BP	391.47	0.15	VP	1966OSB
				BP	391.47	0.01		2019DIK
	neopentanethiol	liq	SEL	BP	376.81	0.15	VP	1966OSB

				BP	376.74	0.09		2019DIK
				BP	376.9			1969LAN
	tert-pentanethiol	liq	SEL	BP	398.16	0.15	VP	1966OSB
				BP	398.15	0.02		2019DIK
$C_6H_{14}S$	1-hexanethiol	liq	SEL	BP	425.81	0.15	VP ebul	1966OSB
				BP	425.80	0.15	BP rev	2019DIK
				BP	425.75	0.15	BP ebul	1960HAI
$C_7H_{16}S$	1-heptanethiol	liq	SEL	BP	450.07	0.15	VP ebul	1966OSB
				BP	450.06	0.15	BP rev	2019DIK
				BP	450.05	0.15	BP ebul	1960HAI
Alkyl Sulfides								
CS_2	carbon disulfide	liq	SEL	BP	319.37	0.15	VP	1962WAD
				BP	319.35	0.15	BP rev	2019DIK
				BP	319.37	0.15	BP rev	2012KRO
				BP	319.37	0.15		1972BOU
				BP	318.35	0.15		1949FEW
$C_2H_6S_2$	dimethyl disulfide	liq	SEL	BP	382.89	0.15	VP	1950SCO
				BP	382.86	0.15	BP rev	2019DIK
				BP	382.89	0.15	VP	1952WHI
C_2H_6S	dimethyl sulfide	liq	SEL	BP	310.45	0.15	VP ebul	1942OSB
				BP	310.47	0.15	BP rev	2019DIK
				BP	310.42	0.15	BP rev	2012KRO
				BP	310.43	0.15	GLC	1957DES
				BP	310.55	0.15	BP ebul	1956HAI
				BP	310.43	0.15	VP	1952WHI
C_3H_8S	ethyl methyl sulfide	liq	SEL	BP	339.80	0.15	VP ebul	1952WHI
				BP	339.76	0.15	BP rev	2019DIK
$C_4H_{10}S$	diethyl sulfide	liq	SEL	BP	365.25	0.15	VP ebul	1966OSB
				BP	365.21	0.15	BP rev	2019DIK
				BP	365.21	0.15	GLC	1957DES
				BP	365.21	0.15	VP	1952WHI
	isopropyl methyl sulfide	liq	SEL	BP	358.0	0.2		1956HAI
				BP	357.88	0.05		2019DIK
				BP	357.8	-	VP	1952WHI
				BP	358.0	-		1951MCA
	methyl isopropyl sulfide	liq		BP	357.88	0.15	BP rev	2019DIK
				BP	358.0	0.2	BP ebul	1956HAI
				BP	357.97	0.15	VP	1952WHI

	methyl propyl sulfide	liq	SEL	BP	368.69	0.15	VP	1952WHI
				BP	368.66	0.15	BP rev	2019DIK
				BP	368.80	0.15	BP ebul	1956HAI
$C_5H_{12}S$	ethyl isopropyl sulfide	liq	SEL	BP	380.4	1.0	VP	1952WHI
				BP	380.50	0.02		2019DIK
				BP	380.5			1951MCA
				BP	376.1			1933ING
	ethyl propyl sulfide	liq	SEL	BP	391.65	0.15	VP	1952WHI
				BP	391.62	0.15	BP rev	2019DIK
				BP	391.65	0.15	GLC	1957DES
$C_6H_{14}S$	di-*n*-propyl sulfide	liq	SEL	BP	415.98	0.15	VP	1952WHI
				BP	415.96	0.15	BP rev	2019DIK
				BP	415.85	0.15	BP ebul	1960HAI
$C_8H_{18}S$	di-*n*-butyl sulfide	liq	SEL	BP	462.06	0.15	VP	1952WHI
				BP	462.06	0.15	BP rev	2019DIK
				BP	461.95	0.15	BP ebul	1960HAI
C_2H_4S	thiacyclopropane	liq	SEL	BP	328.1	0.4	VP	1952GUT
				BP	328.06	0.01		2019DIK
				BP	328.9			1947LEC
Thiacycloalkanes								
C_3H_6S	thiacyclobutane	liq	SEL	BP	368.11	0.15	BP rev	2019DIK
C_4H_8S	thiacyclopentane	liq	SEL	BP	394.27	0.15	VP ebul	1966OSB
				BP	394.26	0.15	BP rev	2019DIK
				BP	393.42	0.15	VP isoten	1971EON
				BP	394.26	0.15		1962DAV
				BP	394.60	0.15	VP	1952WHI
$C_5H_{10}S$	thiacyclohexane	liq	SEL	BP	368.11	0.15	BP rev	2019DIK
Thiacycloalkenes								
C_4H_4S	thiacyclopentadiene	liq	SEL	BP	357.31	0.15	VP	1949WAD
				BP	357.24	0.15	BP rev	2019DIK
				BP	356.52	0.15	VP isoten	1971EON
				BP	357.25	0.15	GLC	1957DES
				BP	357.25	0.15	VP	1952WHI
Aromatic Thiols								
C_6H_6S	benzenethiol	liq	SEL	BP	442.29	0.15	VP ebul	1966OSB
				BP	442.25	0.15	BP rev	2019DIK
				BP	442.25	0.15	BP ebul	1960HAI
Alkyl Sulfoxides								

C_2H_6OS	dimethyl sulfoxide	liq	SEL	BP	463.86	0.20	VP	1972JAK
		sol	SEL1	MP	291.6	0.3	MP	1948DOU
		liq		BP	464.37	0.22	BP rev	2019DIK

HALOGEN-SUBSTITUTED HYDROCARBONS								
Fluoroalkanes								
CH_3F	fluoromethane	gas	SEL	BP	194.8		EOS	2006LEM
				BP	194.89	0.09	BP rev	2019DIK
				BP	194.8		EOS-rev	2018LEM
				BP	195.2			1991PAP
				BP	194.8	1.6	VP	1989HOL
				BP	194.3	1.0		1989FON
				BP	194.86	0.05	VP	1983OI
				BP	195.2			1968FIL
				BP	194.83	0.06	VP	1948MIC
				BP	194.7		BP	1940GRO
CH_2F_2	difluoromethane	gas	SEL	BP	221.499	0.008	EOS	1997TIL
				BP	221.499	0.008	EOS-rev	2018LEM
				BP	221.5		BP rev	2010SYN
				BP	221.4			1997BAR
				BP	221.7	1.0		1994WID
				BP	221.49	0.05		1993WEB
				BP	221.42	0.05		1987KAN
				BP	221.45	0.17		1973LOS
				BP	221.46	0.15	VP	1968MAL
				BP	221.2			1968FIL
				BP	221.6			1964CRO
				BP	221.6			1939HEN
CHF_3	trifluoromethane	gas	SEL	BP	191.3		EOS	2003PEN
				BP	191.09	0.16	BP rev	1982POP
				BP	191.1		EOS-rev	2018LEM
				BP	188.8		BP rev	2010SYN
				BP	191.1			1962VAL
				BP	191.0			1964CRO
				BP	189.0			1962VAL
				BP	190.98	0.15	VP	1962VAL
				BP	191.0	0.5		1959HOU
				BP	191.19	0.05		1971STR
				BP	191.0			1956THO
				BP	189.0			2003PEN
CF_4	tetrafluoromethane	gas	SEL	BP	145.1		EOS	1990PLA
				BP	145.20	0.04	BP rev	2019DIK

				BP	145.1		EOS-rev	2018LEM
				BP	145.21	0.15		2010YU
				BP	145.6	1.0		2007ZHU
				BP	145.23	0.15		1979LOB
				BP	145.56	0.20	VP	1972REG
				BP	145.0			1971STR
				BP	145.1	1.0		1969SMI
				BP	145.2			1968FIL
				BP	145.16	0.20		1968BLA
				BP	145.13	0.25		1967SIM
				BP	145.1			1967GIL
				BP	145.1			1964CRO
				BP	145.34	0.20		1960CHA
				BP	145.1			1956THO
				BP	145.4			1933THO
				BP	145.15	0.15	VP	1933MEN
C_2H_5F	fluoroethane	gas	SEL	BP	235.69	0.15	VP	1975VID
				BP	235.55	0.27	BP rev	2019DIK
				BP	235.61	0.04	EOS-rev	2018LEM
				BP	235.1	0.5		2018HE
				BP	235.61	0.04	EOS	2016QI
				BP	236.1	0.3	BP rev	2010SYN
				BP	235.7	0.4	VLE extrap	2006HAN
				BP	235.7	0.4	VP	2005CHE
				BP	235.9	0.3	VLE	2001KUL
				BP	235.63	0.15	VLE	1998BEY
				BP	236.0			1991PCR
				BP	235.5	0.3		1989WEA
				BP	235.5	0.3	BP	1936GRO
$C_2H_4F_2$	1,1-difluoroethane	gas	SEL	BP	249.13	0.05	EOS	1996OUT
				BP	249.13	0.05	EOS-rev	2018LEM
				BP	248.5		BP rev	2010SYN
				BP	249.1		VP ebul	1993SIL
				BP	246.7	1.0	VP rev	1947STU
				BP	248.5		BP	1936HEN
	1,2-difluoroethane	liq	SEL	BP	304	10		1955EDG
		gas		BP	287	9	BP est	2019DIK
				BP	293.0		BP rev	2012KRO

		liq		BP	303.9			2010SYN
				BP	304.5			1960KLA
		gas		BP	283.7		BP	1936HEN
$C_2H_3F_3$	1,1,1-trifluoroethane	gas	SEL	BP	225.91	0.04	EOS	2000LEM
				BP	225.92	0.18	BP rev	2019DIK
				BP	225.91	0.04	EOS-rev	2018LEM
				BP	225.6		BP rev	2010SYN
				BP	226.2		VLE	2001KUL
				BP	226		BP rev	1990PCR
				BP	225.8	0.4	VP	1944RUS
				BP	226.5		BP	1936HEN
				BP	226.4			1933SWA
	1,1,2-trifluoroethane	gas		BP	276.8	0.3	BP rev	2019DIK
				BP	278.2		BP rev	2010SYN
				BP	276.1			1940YOU
			SEL	BP	278.2	1.0	BP	1936HEN
$C_2H_2F_4$	1,1,1,2-tetrafluoroethane	gas	SEL	BP	247.076	0.009	EOS	1994TIL
				BP	247.07	0.22	BP rev	2019DIK
				BP	247.076	0.009	EOS-rev	2018LEM
				BP	247.1	0.5	VLE	2011DON
				BP	246.7		BP rev	2010SYN
				BP	247.0	0.1	VLE	1996BLA
				BP	247.076	0.004	EOS	1994TIL
				BP	247.02	0.22	VLE	1992GOO
				BP	246.6		BP rev	1990PCR
				BP	247.15	0.25	VLE	1990NIS
				BP	248.5		quote	1963EDG
	1,1,2,2-tetrafluoroethane	gas	SEL	BP	253.23	0.15	VP	1991MAE
				BP	253.44	0.12	BP rev	2019DIK
				BP	253.7		BP rev	2010SYN
				BP	250.15	0.08	VP rev	1979KUD
				BP	250.2			1959EIS
				BP	250.2		VP	1940YOU
C_2HF_5	pentafluoroethane	gas	SEL	BP	225.06	0.04	EOS	2005LEM
				BP	225.06	0.04	EOS-rev	2018LEM
				BP	225.3	0.7	VP	2001KUL
				BP	224.6		BP	1999TAK
				BP	225.1	0.2	BP	1997BAR

				BP	225.05	0.07	VP	1994WEB
				BP	224.83	0.23	VP	1992WIL
				BP	224.7	1.0	BP	1968FIL
				BP	225.2	1.0	BP	1952CUC
C_2F_6	hexafluoroethane	gas	SEL	BP	195.06	0.06	EOS	2006LEM
				BP	195.06	0.06	BP rev	2019DIK
				BP	195.06	0.06	EOS-rev	2018LEM
				BP	194.87	0.20	VP	1948PAC
Fluoroalkenes								
C_2H_3F	fluoroethene	gas	SEL	BP	201.7	0.5	VP rev	1947STU
				BP	201	14	BP est	2019DIK
$C_2H_2F_2$	1,1-difluoroethene	gas	SEL	BP	187.6	1.2	BP rev	2019DIK
				BP	190.2		BP rev	2010SYN
				BP	190.2		BP rev	1989WEA
	1,2-difluoroethene, (*E*)-	gas	SEL	BP	221	20	BP est	2019DIK
				BP	231		BP rev	2010SYN
	1,2-difluoroethene, (*Z*)-	gas	SEL	BP	220	21	BP rev	2019DIK
				BP	253		BP rev	2010SYN
C_2HF_3	trifluoroethene	gas	SEL	BP	211.7	1.5	BP	1961CRA
				BP	211.8	0.6	BP rev	2019DIK
				BP	220.2		BP comp	2001HOR
				BP	222		BP rev	1990PCR
				BP	212.7		BP	1953PRO
C_2F_4	tetrafluoroethene	gas	SEL	BP	197.51	0.25	VP	1953FUR
				BP	197.57	0.04	BP rev	2019DIK
				BP	199.2		BP	1953LAZ
				BP	196.7		BP	1953ATK
				BP	196.9		VP	1946REN
				BP	196.8		VP	1933RUF
Chloroalkanes								
CH_3Cl	chloromethane	gas	SEL	BP	248.99	0.15	VLE	1948GAN
				BP	249.01	0.07	BP rev	2019DIK
				BP	249.0	0.3	VP	1988HOL
				BP	249.1			1966GAL
				BP	249.31	0.15	VP	1947BEE
				BP	249.4			1943MCG
CH_2Cl_2	dichloromethane	liq	SEL	BP	312.92	0.15	VLE	1960MUE
				BP	312.96	0.04	BP rev	2019DIK

				BP	312.9		VLE	1990KRI
				BP	312.9			1972BOU
				BP	312.9			1950MUM
				BP	313.34	0.25	VLE	1948GAN
$CHCl_3$	trichloromethane	liq	SEL	BP	334.42	0.18	VP rev	1947STU
				BP	334.31	0.05	BP rev	2019DIK
CCl_4	tetrachloromethane	liq	SEL	BP	349.88	0.05	VP ebul	1959HIL
				BP	349.86	0.07	BP rev	2019DIK
				BP	349.7		BP rev	2010SYN
C_2H_5Cl	chloroethane	gas	SEL	BP	285.40	0.15	VP	1948GOR
				BP	285.45	0.06	BP rev	2019DIK
$C_2H_4Cl_2$	1,1-dichloroethane	liq	SEL	BP	330.42	0.15	VP	1956LI
				BP	330.35	0.03	BP rev	2019DIK
				BP	330.2		VLE	1999IGO
				BP	330.4		VLE	1988WIS2
				BP	330.3		VLE	1985KOV
				BP	330.4		VLE	1951NEW
	1,2-dichloroethane	liq	SEL	BP	356.70	0.20	VLE	1996KRI
				BP	356.58	0.15	BP rev	2019DIK
				BP	356.65	0.03	EOS-rev	2018LEM
				BP	356.58	0.08	VP	2008AMI
				BP	356.7		VLE	1989MAT
				BP	356.6		VLE	1986PAU2
				BP	356.61	0.13	VP	1951SIE
				BP	356.62	0.08	VP	1943E.W
				BP	356.98	0.15	VP	1929PEA
$C_2H_3Cl_3$	1,1,1-trichloroethane	liq	SEL	BP	347.35	0.20	BP ebul	1985RED
				BP	347.22	0.07	BP rev	2019DIK
				BP	347.4		VLE	2007RAD
				BP	347.0		VLE	2005KUM
				BP	347.0	0.3	VLE	1996KRI
				BP	346.7		VLE	1995COM
				BP	347.2		VLE	1982VIS
				BP	341.0		VP extrap	1944RUB
	1,1,2-trichloroethane	liq	SEL	BP	386.82	0.10	VP rev	1949DRE2
				BP	386.74	0.08	BP rev	2019DIK
				BP	386.8			1967HAN
				BP	387.2		BP rev	1955TIM

$C_2H_2Cl_4$	1,1,1,2-tetrachloroethane	liq	SEL	BP	403.3	0.3	VP rev	1949DRE2
				BP	403.33	0.05	BP rev	2019DIK
				BP	403.0	0.4	VLE	1985KOV
	1,1,2,2-tetrachloroethane	liq	SEL	BP	422.3	1.0	VP	1950MAT
				BP	419.1	0.6	BP rev	2019DIK
				BP	419.25	0.15	VLE	1996KRI
				BP	419.4		BP ebul	1985RED
C_2HCl_5	pentachloroethane	liq	SEL	BP	435.1	0.3	VLE	1988MIH
				BP	435	5	BP rev	2019DIK
				BP	433.6		BP rev	1943MCG
				BP	435.1		BP	1941EWE
				BP	434.6			1935EAR
				BP	441.6	2.0	BP	1930NEL
				BP	435.1		VLE	1926LEC
C_2Cl_6	hexachloroethane	sol	SEL	MP	460.0	2.0	MP	1962SHA
		liq		BP	463.0	0.5	VP rev	1947STU
				BP	458.2		VP extrap	2019DIK
		sol		MP	458.9	0.3	MP	1956MIL
Chloroalkenes								
C_2H_3Cl	chloroethene	gas	SEL	BP	259.35	0.05	VP ebul	1959MCD
				BP	259.40	0.05	BP rev	2019DIK
				BP	259.44	0.07	EOS-rev	2018LEM
$C_2H_2Cl_2$	1,1-dichloroethene	liq	SEL	BP	304.71	0.05	VP ebul	1959HIL2
				BP	304.69	0.04	BP rev	2019DIK
				BP	304.55	0.15	VLE	1985KOV2
				BP	304.8		VLE	1981EFR
	1,2-dichloroethene, (*E*)-	liq	SEL	BP	320.73	0.25	VP	1947KET
				BP	320.8	0.6	BP rev	2019DIK
				BP	320.8		VLE	1985MAC
				BP	320.5		VLE	1985KOV2
				BP	321.4		VLE	1951NEW
				BP	321.9		VLE	1951FLO
	1,2-dichloroethene, (*Z*)-	liq	SEL	BP	333.6	0.5	VP	1947KET
				BP	333.32	0.21	BP rev	2019DIK
				BP	333.2			1951AND
				BP	333.5		BP	1941MAR
C_2HCl_3	trichloroethene	liq	SEL	BP	360.5	0.4	VP isoten	1944MCD
				BP	359.84	0.11	BP rev	2019DIK

C_2Cl_4	tetrachloroethene	liq	SEL	BP	394.29	0.15	VLE	1970POL
				BP	394.25	0.10	BP rev	2019DIK
Chloroacetylenes								
C_2HCl	chloroacetylene	gas	SEL	BP	238	10	BP rev	1987STE
				BP	243		explod	2021EPA
				BP	243	9	predict	2021CHE
C_2Cl_2	dichloroacetylene	sol	SEL	explod	306	10	explod	2021EPA
		liq		BP	365	15	BP rev	2012KRO
				BP	306		BP rev	1999LEW
				BP	306	10		1967SMI
Chloroaromatics								
C_6H_5Cl	chlorobenzene	liq	SEL	BP	405.21	0.25	EOS-rev	2018LEM
				BP	404.7	0.3	BP eval	2019DIK
				BP	404.6	0.5	VLE	1995KRI
				BP	405.2	0.5	VLE	1990JOS
				BP	404.9	0.5	VLE	1989RED
				BP	405.0	0.5	VLE	1988AQU
Bromoalkanes								
CH_3Br	bromomethane	gas	SEL	BP	276.70	0.15	VP	1947BEE
				BP	276.66	0.15	BP rev	2019DIK
				BP	276.7	0.1	VP rev	1979KUD
CH_2Br_2	dibromomethane	liq	SEL	BP	370.1	0.1	VP rev	1979KUD
				BP	370.1	0.5	BP rev	2019DIK
				BP	371.7	1.0	VP rev	1947STU
$CHBr_3$	tribromomethane	liq	SEL	BP	422.36	0.05	VP rev	1979KUD
				BP	422.37	0.23	BP rev	2019DIK
				BP	421.83	0.25	VLE	1941SIM
CBr_4	tetrabromomethane	sol	SEL	MP	367.6	2.0	MP	1970SIL
		liq	SEL1	BP	462.6	0.6	BP rev	1979KUD
				BP	462.7		BP comp	2021EPA
				BP	462.6	1.0	VP rev	1947STU
C_2H_5Br	bromoethane	liq	SEL	BP	311.54	0.19	VP	1930ZMA
				BP	311.5	0.4	BP rev	2019DIK
$C_2H_4Br_2$	1,2-dibromoethane	liq	SEL	BP	404.56	0.10	VP rev	1949DRE
				BP	404.58	0.06	BP rev	2019DIK
Bromoalkenes								
C_2H_3Br	bromoethene	liq	SEL	BP	306	18	BP est	2019DIK
		gas		BP	288.6	0.5	VP	1937GUY

Iodoalkanes								
CH_3I	iodomethane	liq	SEL	BP	315.58	0.02	VP rev	1979KUD
				BP	315.58	0.09	BP rev	2019DIK
Chlorofluoromethanes								
CH_2ClF	chlorofluoromethane	gas	SEL	BP	264.1	1.0	BP rev	1979KUD
				BP	260	13	BP est	2019DIK
				BP	264.1		BP rev	2010SYN
				BP	264			1990PCR
$CHClF_2$	chlorodifluoromethane	gas	SEL	BP	232.32	0.02	VP rev	1979KUD
				BP	232.34	0.03	BP rev	2019DIK
				BP	232.4		BP rev	2010SYN
				BP	232.28	0.15	VP	1964KLE
$CHCl_2F$	dichlorofluoromethane	gas	SEL	BP	282.05	0.10	VP rev	1979KUD
				BP	282.01	0.09	BP rev	2019DIK
				BP	282.0	0.8	EOS-rev	2018LEM
				BP	282.0	0.8	EOS	2015PLA
				BP	282.1		BP rev	2010SYN
				BP	282.3	0.2	VP rev	1947STU
$CHClF_2$	difluorochloromethane	gas	SEL	BP	232.32	0.12	VP rev	1979KUD
				BP	232.34	0.03	BP rev	2019DIK
$CsClF_3$	chlorotrifluoromethane	gas	SEL	BP	191.7	0.1	VP rev	1979KUD
				BP	191.75	0.04	BP rev	2019DIK
				BP	191.67	0.02	EOS-rev	2018LEM
				BP	191.8		BP rev	2010SYN
				BP	191.67	0.02	EOS	2000MAG
				BP	191.91	0.18	VP rev	1947STU
CCl_2F_2	dichlorodifluoromethane	gas	SEL	BP	243.38	0.04	VP rev	1979KUD
				BP	243.42	0.05	BP rev	2019DIK
				BP	243.40	0.05	EOS-rev	2018LEM
				BP	243.4		BP rev	2010SYN
				BP	243.40	0.05	EOS	1992MAR
				BP	243.29	0.18	VP rev	1947STU
CCl_3F	trichlorofluoromethane	gas	SEL	BP	296.78	0.02	VP rev	1979KUD
				BP	296.84	0.06	BP rev	2019DIK
				BP	296.86	0.06	EOS-rev	2018LEM
				BP	297.0		BP rev	2010SYN
				BP	296.858	0.056	EOS	1992JAC
				BP	296.78	0.06	VP ebul	1941OSB

				BP	296.86	0.10	VP	1940BEN
Chlorofluoroethanes								
C_2H_4ClF	1-chloro-1-fluoroethane	gas	SEL	BP	289.3	1.5	BP	1936HEN
				BP	289.3	1.5	BP est	2019DIK
				BP	289.3		BP rev	2010SYN
$C_2H_3Cl_2F$	1,1-dichloro-1-fluoroethane	liq	SEL	BP	305.26	0.25	VP	1991MAE
				BP	305.222	0.024	BP rev	2019DIK
				BP	305.2		BP rev	2010SYN
				BP	304.7		VP	1997DUA
				BP	305.60	0.15	VP	1993DEF
				BP	305.4		VP ebul	1992WEB
				BP	305.10	0.25	BP	1943HEN
				BP	304.9		BP	1936HEN
	1,2-dichloro-1-fluoroethane	liq	SEL	BP	346.95	0.15	BP	1936HEN
				BP	346.9	1.9	BP est	2019DIK
				BP	349.2		BP rev	2010SYN
$C_2H_3ClF_2$	1-chloro-1,1-difluoroethane	gas	SEL	BP	264.04	0.25	VP ebul	1993SIL
				BP	264.04	0.24	BP rev	2019DIK
				BP	264.0		BP rev	2010SYN
				BP	263.6		BP	1936HEN
	1-chloro-2,2-difluoroethane	liq	SEL	BP	308.25	0.15	BP	1936HEN
				BP	309.2		BP rev	2010SYN
$C_2H_2ClF_3$	2-chloro-1,1,1-trifluoroethane	gas	SEL	BP	279.25	0.15	VP	1936HEN
				BP	279.19	0.22	BP rev	2019DIK
				BP	280.1		BP rev	2010SYN
Chlorofluoroalkenes								
C_2HCl_2F	1,2-dichloro-1-fluoroethene	liq	SEL	BP	305.7	2.5	BP rev	2010SYN
				BP	308		BP rev	1990PCR
C_2ClF_3	chlorotrifluoroethene	gas	SEL	BP	244.8	0.1	VP	1951OLI
				BP	244.85	0.19	BP rev	2019DIK
				BP	246			1990PCR
				BP	244.7		BP rev	1990ALD
				BP	246.0			1982ERA
Bromofluoroalkanes								
CH_2BrF	bromofluoromethane	gas	SEL	BP	290.7	2.0	BP rev	1979KUD
		liq		BP	310	12	BP est	2019DIK
				BP	310.0		BP rev	2012KRO
		gas		BP	290.7		BP rev	2010SYN

				BP	292.2		VP rev	1999DYK
$CHBrF_2$	bromodifluoromethane	gas	SEL	BP	257.5	0.2	VP rev	1979KUD
				BP	257.5	0.4	BP rev	2019DIK
				BP	258.7		BP rev	2010SYN
$CHBr_2F$	dibromofluoromethane	liq	SEL	BP	337	2	BP rev	1979KUD
				BP	351	13	BP est	2019DIK
				BP	338.1		BP rev	2010SYN
$CBrF_3$	bromotrifluoromethane	gas	SEL	BP	215.26	0.05	VP ebul	1959MCD
				BP	215.32	0.08	BP rev	2019DIK
				BP	215.4		BP rev	2010SYN
				BP	215.3	0.3	VP rev	1979KUD
CBr_2F_2	dibromodifluoromethane	gas	SEL	BP	295.93	0.04	VP rev	1979KUD
				BP	295.94	0.04	BP rev	2019DIK
				BP	297.7		BP rev	2010SYN
				BP	295.94	0.05	VP ebul	1959MCD
CBr_3F	tribromofluoromethane	liq	SEL	BP	379.6	1.0	BP rev	1979KUD
				BP	404	17	BP est	2019DIK
				BP	379.7		BP rev	2010SYN
Bromochloroalkanes								
CH_2BrCl	bromochloromethane	liq	SEL	BP	341.21	0.08	VP rev	1979KUD
				BP	341.12	0.04	BP rev	2019DIK
				BP	341.22	0.05	VP ebul	1959MCD
$CHBrCl_2$	bromodichloromethane	liq	SEL	BP	363.3	0.4	BP rev	1979KUD
				BP	363	3	BP est	2019DIK
				BP	362.7		BP rev	2010SYN
$CHBr_2Cl$	dibromochloromethane	liq	SEL	BP	393	2	BP rev	1979KUD
				BP	405	13	BP est	2019DIK
$CBrCl_3$	bromotrichloromethane	liq	SEL	BP	378.1	1.0	VP rev	1979KUD
				BP	378	3	BP est	2019DIK
				BP	376	4	BP rev	2012KRO
				BP	376.7		BP	1950ZAK
CBr_2Cl_2	dibromodichloromethane	liq	SEL	BP	393	2	BP rev	1979KUD
				BP	423.2			2021EPA
				BP	414	22	BP est	2019DIK
				BP	423.4		BP rev	2014HAY
				BP	329.9		BP rev	1955VAR
CBr_3Cl	tribromochloromethane	liq	SEL	BP	433	1	BP rev	1979KUD
				BP	452	18	BP est	2019DIK

Bromochlorofluoroalkanes								
$CHBrClF$	bromochlorofluoromethane	liq	SEL	BP	309	2	BP rev	1979KUD
				BP	313	16	BP est	2019DIK
				BP	309.7		BP	1952HAS
				BP	309.3	1.0	BP	1942BER
$CBrClF_2$	bromochlorodifluoromethane	gas	SEL	BP	269.14	0.04	VP rev	1979KUD
				BP	269.24	0.03	BP rev	2019DIK
				BP	270.7		BP rev	2010SYN
				BP	269.19	0.15	VP	1960GLE
$CBrCl_2F$	bromodichlorofluoromethane	liq	SEL	BP	323	15	VP	1979KUD
				BP	338	20	BP est	2019DIK
				BP	325		BP rev	2010SYN
				BP	323.6			1957MIL
CBr_2ClF	dibromochlorofluoromethane	liq	SEL	BP	353	2	BP rev	1979KUD
				BP	376	19	BP est	2019DIK
				BP	353		BP rev	2010SYN
				BP	353.2	1.0	BP	1952HAS
Carbonyl Halides								
$CHFO$	carbonyl fluoride	gas	SEL	BP	245.2	2.0	VP	1964FIS
CF_2O	carbonyl difluoride	gas	SEL	BP	188.58	0.20	VP	1968PAC
CCl_2O	phosgene	gas	SEL	BP	280.71	0.15	VP	1948GIA
				BP	280.66	0.17	BP rev	2019DIK
Chlorophenols								
C_6HCl_5O	pentachlorophenol	liq	SEL	BP	583	3	VP	1947STU
		sol	SEL1	MP	462.8	1.0	MP	1959MCD
		liq		BP	588	19	BP est	2019DIK
		sol		MP	463.8	1.0	MP	1990DON

Siloxanes								
$C_6H_{18}OSi_2$	hexamethyldisiloxane	liq	SEL	BP	373.66	0.10	VP	1961SCO
$C_8H_{24}O_4Si_4$	octamethylcyclotetrasiloxane	liq	SEL	BP	448.9	0.6	EOS	2016THO
		sol	SEL1	MP	290.7	1.0	MP	1968MAR
		liq		BP	446.2	2.0	VLE	1959MYE
				BP	448.0	1.0	VP	1954OST

2.3. Recommended Melting and Boiling Points

Table 2-2 provides the selected recommended values for melting and boiling points, while all values that were compiled are given previously in Table 2-1. This table is divided into several sub-tables by compound class. Within each sub-table the compounds are ordered by secondary class and then by molecular formula. All references for melting and boiling point data provided in the last subsection 2.4.

Table 2-3. Recommended Melting and Boiling Points

Table 2-3(1). Small Molecules

Formula	Compound	Phase	SEL	trs	T_{trs}/K	unc/K	Method	Reference
Hydrogen/Oxygen								
H_2	hydrogen	gas	SEL	BP	20.369	0.014	EOS	2009LEA
O_2	oxygen	gas	SEL	BP	90.188	0.029	EOS	1991STE
H_2O	water	liq	SEL	BP	373.124	0.014	EOS	1995WAG
		sol	SEL1	MP	273.153	0.001	EOS	2006FEI
			SEL2	TP	273.16	0.01	DEF	1990PRE
H_2O_2	hydrogen peroxide	liq	SEL	BP	426.31	0.05	VLE rev	2004MAN
		sol	SEL1	MP	272.69	0.02	SLE	1951FOL
			SEL2	TP	272.74	0.05	TP	1954GIG
Nitrogen/Hydrogen								
N_2	nitrogen	gas	SEL	BP	77.355	0.007	EOS	2000SPA
H_3N	ammonia	gas	SEL	BP	239.823	0.020	EOS	2018GAO
H_4N_2	hydrazine	liq	SEL	BP	386.7	0.9	BP	1989TIP
HN_3	hydrogen azide	liq	SEL	BP	308.9	1.5	BP rev	2007LID
Nitrogen/Oxygen								
N_2O	nitrous oxide	gas	SEL	BP	184.68	0.07	EOS	2006LEM
ClH_4NO_4	ammonium perchlorate	sol	SEL	dec	595.9	4.0	DTA	2004LIU
			SEL	TP	513.2	1.0	TP rev	2019DIK
Sulfur/Hydrogen/Oxygen								
H_2S	hydrogen sulfide	gas	SEL	BP	212.85	0.10	EOS	2006LEM
O_2S	sulfur dioxide	gas	SEL	BP	263.14	0.09	EOS	2016GAO

Boron/Hydrogen/Oxygen								
B_2H_6	diborane	gas	SEL	BP	180.6	0.1	VP	1959PAR
Hydrogen Halides								
ClH	hydrogen chloride	gas		BP	188.173	0.088	EOS	2018THO

Table 2-3(2). Hydrocarbons

Formula	Compound	Phase	SEL	trs	T_{trs}/K	unc/K	Method	Reference
Carbon								
C	graphite	sol	SEL	MP	4800	100	MP rev	2005SAV
Alkanes								
CH_4	methane	gas	SEL	BP	111.667	0.013	EOS	1991SET
C_2H_6	ethane	gas	SEL	BP	184.566	0.004	EOS	2006BUC
C_3H_8	propane	gas	SEL	BP	231.039	0.009	EOS	2009LEM
C_4H_{10}	isobutane	gas	SEL	BP	261.40	0.26	EOS	2006BUC2
	n-butane	gas	SEL	BP	272.66	0.12	EOS	2006BUC2
C_5H_{12}	isopentane	liq	SEL	BP	301.0	0.7	EOS	2006LEM
	neopentane	gas	SEL	BP	282.650	0.028	EOS	2006LEM
	n-pentane	liq	SEL	BP	309.21	0.12	EOS	2018THO
C_6H_{14}	2,3-dimethylbutane	liq	SEL	BP	331.088	0.070	VP	1945WIL
	3-methylpentane	liq	SEL	BP	336.43	0.07	VP	1945WIL
	isohexane	liq	SEL	BP	333.36	0.06	EOS	2006LEM
	neohexane	liq	SEL	BP	322.85	0.13	EOS-rev	2018LEM
	n-hexane	liq	SEL	BP	341.87	0.13	EOS	2018THO2
C_7H_{16}	2,2,3-trimethylbutane	liq	SEL	BP	354.03	0.10	VP	1949FOR
	2,3-dimethylpentane	liq	SEL	BP	362.93	0.06	VLE	1974OSB
	2,4-dimethylpentane	liq	SEL	BP	353.7	0.3	VLE	1976TRI
	3,3-dimethylpentane	liq	SEL	BP	359.21	0.10	VP	1949FOR
	3-methylhexane	liq	SEL	BP	365.00	0.10	VP	1949FOR
	isoheptane	liq	SEL	BP	363.20	0.15	VP	1949FOR
	neoheptane	liq	SEL	BP	352.25	0.15	BP rev	1947FEN
	n-heptane	liq	SEL	BP	371.55	0.07	EOS	2018TEN
C_8H_{18}	2,2,4-trimethylpentane	liq	SEL	BP	372.36	0.14	EOS	2018BLA
	2,2-dimethylhexane	liq	SEL	BP	379.74	0.07	VP	1945WIL
	2-methylheptane	liq	SEL	BP	390.90	0.15	BP rev	1947FEN
	n-octane	liq	SEL	BP	398.79	0.14	EOS	2018BEC
C_9H_{20}	isononane	liq	SEL	BP	416.41	0.15		1950MEA
	neononane	liq	SEL	BP	403.65	0.15	BP rev	1947FEN
	n-nonane	liq	SEL	BP	423.91	0.15	EOS	2006LEM
$C_{10}H_{22}$	*n*-decane	liq	SEL	BP	447.27	0.16	EOS	2006LEM
$C_{11}H_{24}$	*n*-undecane	liq	SEL	BP	469.05	0.15	BP rev	1947FEN
$C_{12}H_{26}$	*n*-dodecane	liq	SEL	BP	489.44	0.08	EOS	2004LEM
		sol	SEL1	MP	263.5	0.2	MP	1983OTT

			SEL2	TP	263.6		EOS	2004LEM
$C_{16}H_{34}$	*n*-hexadecane	liq	SEL	BP	559.9	0.2		2018LEM
		sol	SEL1	MP	291.3	0.1	MP	1986SNO
			SEL2	TP	291.3			2018LEM
Alkenes								
C_2H_4	ethene	gas	SEL	BP	169.38	0.02	EOS	2000SMU
C_3H_6	propene	gas	SEL	BP	225.53	0.04	EOS-rev	2018LEM
C_4H_8	1-butene	gas	SEL	BP	266.83	0.15	VLE	1976STE
	2-butene, (E)-	gas	SEL	BP	274.01	0.15	VP	1945GUT
	2-butene, (Z)-	gas	SEL	BP	276.87	0.08	VP	1944SCO
	isobutene	gas	SEL	BP	266.05	0.15	VP	1940LAM
C_5H_{10}	1-pentene	liq	SEL	BP	303.12	0.08	VP	1949SCO
	2-methyl-1-butene	liq	SEL	BP	304.30	0.13	VP	1949SCO
	2-methyl-2-butene	liq	SEL	BP	311.72	0.15	VP	1949SCO
	2-pentene, (E)-	liq	SEL	BP	309.51	0.08	VP	1950SCO2
	2-pentene, (Z)-	liq	SEL	BP	310.09	0.08	VP	1950SCO2
	3-methyl-1-butene	gas	SEL	BP	293.21	0.08	VP	1950SCO2
C_6H_{12}	1-hexene	liq	SEL	BP	336.64	0.06	VP	1950FOR
C_7H_{14}	1-heptene	liq	SEL	BP	366.71	0.06	VP	1950FOR
C_8H_{16}	1-octene	liq	SEL	BP	394.43	0.06	VP	1950FOR
C_9H_{18}	1-nonene	liq	SEL	BP	420.02	0.06	VP	1950FOR
$C_{10}H_{20}$	1-decene	liq	SEL	BP	443.72	0.06	VP	1950FOR
Alkadienes								
C_3H_4	allene	gas	SEL	BP	238.3	0.5	VP rev	1947STU
C_4H_6	1,2-butadiene	gas	SEL	BP	284.1	0.4		1946STR
	1,3-butadiene	gas	SEL	BP	268.44	0.15	VLE	1976STE
C_5H_8	1,2-pentadiene	liq	SEL	BP	318.01	0.06	VP	1950FOR
	1,3-pentadiene	liq	SEL	BP	314.9	1.5		1956BUS
	1,4-pentadiene	liq	SEL	BP	299.12	0.15	VP	1950FOR
	2-methyl-1,3-butadiene	liq	SEL	BP	307.19	0.15	VLE	1985HOW
Alkynes								
C_2H_2	acetylene	gas	SEL	BP	188.26	0.15	EOS-rev	2018LEM
		sol	SEL1	TP	191.75	0.15	EOS-rev	2018LEM
C_3H_4	propyne	gas	SEL	BP	249.80	0.15	VP	1967VAN
C_4H_6	1-butyne	gas	SEL	BP	281.18	0.15	VP	1950AST
	2-butyne	liq	SEL	BP	300.1	0.2		1954POM2
C_5H_8	1-pentyne	liq	SEL	BP	313.5	0.3	VLE	2021TSU
	2-pentyne	liq	SEL	BP	329.3	0.2		1954POM2

C_6H_{10}	1-hexyne	liq	SEL	BP	344.5	0.2	VLE	2021TSU
	2-hexyne	liq	SEL	BP	357.6	0.2	VLE	2021TSU
	3-hexyne	liq	SEL	BP	354.6	0.3		1954POM2
C_7H_{12}	1-heptyne	liq	SEL	BP	372.9	0.3	BP	1945HEN
C_8H_{14}	1-octyne	liq	SEL	BP	399.4	0.3	BP	1945HEN
Alkenynes								
C_4H_4	butenyne	gas	SEL	BP	276.2	2.0		1954HEN
C_5H_6	1-penten-3-yne	liq	SEL	BP	332.4			1933JAC
	3-penten-1-yne	liq	SEL	BP	317.1	3.0		1954POM2
Alkadiynes								
C_4H_2	butadiyne	gas	SEL	BP	283.7	1.0		1954POM2
Cycloalkanes								
C_3H_6	cyclopropane	gas	SEL	BP	241.7	0.4	EOS	1992POL
C_4H_8	cyclobutane	gas	SEL	BP	285.6	0.2	VP	1953RAT
C_5H_{10}	cyclopentane	liq	SEL	BP	322.40	0.06	EOS	2015GED
	methylcyclobutane	liq	SEL	BP	310	2		1953PIN
C_6H_{12}	cyclohexane	liq	SEL	BP	353.87	0.03	EOS	2014ZHO
	methylcyclopentane	liq	SEL	BP	344.96	0.07	VP	1945WIL
C_7H_{14}	1,1-dimethylcyclopentane	liq	SEL	BP	360.99	0.10	VP	1949FOR
	cycloheptane	liq	SEL	BP	391.92	0.08	VP	1956FIN
	ethylcyclopentane	liq	SEL	BP	376.61	0.10	VP	1949FOR
	methylcyclohexane	liq	SEL	BP	374.12	0.15	VLE	1991AIZ
C_8H_{16}	ethylcyclohexane	liq	SEL	BP	405.05	0.15	BP rev	1935LES
	isopropylcyclopentane	liq	SEL	BP	399.57	0.06	VP	1949FOR
	n-propylcyclopentane	liq	SEL	BP	404.10	0.06	VP	1949FOR
C_9H_{18}	isopropylcyclohexane	liq	SEL	BP	427.71	0.10	VP	1949FOR
	propylcyclohexane	liq	SEL	BP	429.87	0.10	VP	1949FOR
$C_{10}H_{20}$	1,3-diethylcyclohexane	liq	SEL	BP	445.7	1.5		1962ALL
	isobutylcyclohexane	liq	SEL	BP	444.47	0.07	VP	1949FOR
	tert-butylcyclohexane	liq	SEL	BP	444.74	0.10	VP	1949FOR
Cycloalkenes								
C_3H_4	cyclopropene	gas	SEL	BP	237.6	1.5	BP	1941SCH
C_4H_6	cyclobutene	gas	SEL	BP	275.74	0.15	VP	1941HEI
C_5H_8	cyclopentene	liq	SEL	BP	317.39	0.06	VP	1950FOR
	methylenecyclobutane	liq	SEL	BP	315.35	0.15	BP rev	1947FEN
C_6H_{10}	3-methylcyclopentene	liq	SEL	BP	338	1	BP	1945CRA
	cyclohexene	liq	SEL	BP	356.10	0.04	VP	1973MEY
C_7H_{12}	1-ethylcyclopentene	liq	SEL	BP	379.6	0.2		1959PIN

	1-methylcyclohexene	liq	SEL	BP	383.42	0.15	VP	1960CAM
	3-ethylcyclopentene	liq	SEL	BP	371.3		BP	1945CRA
	cycloheptene	liq	SEL	BP	386.1	0.5	GLC	1958TUR
	methylenecyclohexane	liq	SEL	BP	376.58	0.04	VP	1973MEY
C_8H_{14}	1,2-dimethylcyclohexene	liq	SEL	BP	409	2	BP	1938CHI
	1-ethylcyclohexene	liq	SEL	BP	410.11	0.05	VP	1960CAM
Cycloalkadienes								
C_4H_4	cyclobutadiene	gas	SEL	BP	286	12	BP est	2019DIK
C_5H_6	1,3-cyclopentadiene	liq	SEL	BP	313.4	0.2	VP	1965HUL
C_6H_8	1,3-cyclohexadiene	liq	SEL	BP	353.49	0.04	VP	1973MEY
	1,4-cyclohexadiene	liq	SEL	BP	362.66	0.05		1989STE
C_8H_{12}	1,5-cyclooctadiene	liq	SEL	BP	421.8	2.0		1985TAS
Bicycloalkanes								
$C_{10}H_{18}$	*cis*-decalin	liq	SEL	BP	468.93	0.10	VP	1955CAM
	trans-decalin	liq	SEL	BP	460.42	0.10	VP	1955CAM
$C_{12}H_{22}$	cyclohexylcyclohexane	liq	SEL	BP	511.1	0.3	VP	1980WIE
		sol	SEL1	MP	277.2	0.5	MP	1983O'R

Table 2-3(3). Aromatic Hydrocarbons

Formula	Compound	Phase	SEL	trs	T_{trs}/K	unc/K	Method	Reference
Alkylbenzenes								
C_6H_6	benzene	liq	SEL	BP	353.22	0.13	EOS	2012THO
		sol	SEL1	MP	278.67	0.02	MP	1996LIN
C_7H_8	toluene	liq	SEL	BP	383.75	0.04	EOS	2006LEM
		sol	SEL1	MP	178.2	0.2	MP	1998KIM
C_8H_{10}	1,2-dimethylbenzene	liq	SEL	BP	417.56	0.07	VP	1945WIL
	1,3-dimethylbenzene	liq	SEL	BP	412.25	0.07	VP	1945WIL
	1,4-dimethylbenzene	liq	SEL	BP	411.47	0.05	EOS	2012ZHO
	ethylbenzene	liq	SEL	BP	408.96	0.15	VP	1967AMB
C_9H_{12}	1,2,3-trimethylbenzene	liq	SEL	BP	449.23	0.15	VP	1967AMB
	1,2,4-trimethylbenzene	liq	SEL	BP	442.50	0.15	VP	1967AMB
	1,3,5-trimethylbenzene	liq	SEL	BP	437.87	0.15	VP	1967AMB
	2-ethyltoluene	liq	SEL	BP	438.25	0.15	VP	1949FOR
	3-ethyltoluene	liq	SEL	BP	434.46	0.10	VP	1949FOR
	4-ethyltoluene	liq	SEL	BP	435.14	0.10	VP	1949FOR
	isopropylbenzene	liq	SEL	BP	425.54	0.20	VLE	1989CEP
	n-propylbenzene	liq	SEL	BP	432.37	0.15	VP	1967AMB
$C_{10}H_{14}$	1,2-diethylbenzene	liq	SEL	BP	456.57	0.10	VP	1949FOR
	1,3-diethylbenzene	liq	SEL	BP	454.25	0.15	VP	1949FOR
	1,4-diethylbenzene	liq	SEL	BP	456.90	0.10	VP	1949FOR
	2-isopropyltoluene	liq	SEL	BP	451.50	0.15	BP rev	1947FEN
	3-isopropyltoluene	liq	SEL	BP	448.4	0.4		1949BIR
	4-isopropyltoluene	liq	SEL	BP	450.27	0.05	VP ebul	1959MCD
	Isobutylbenzene	liq	SEL	BP	445.95	0.15	BP rev	1947FEN
	n-butylbenzene	liq	SEL	BP	456.42	0.10	VP	1949FOR
	sec-butylbenzene	liq	SEL	BP	446.30	0.15	BP rev	1947FEN
	tert-butylbenzene	liq	SEL	BP	442.27	0.15	VP	1949FOR
Alkenylbenzenes								
C_8H_8	ethenylbenzene	liq	SEL	BP	418.5	0.3		1950BOO
Benzocycloalkanes								
C_9H_{10}	benzocyclopentane	liq	SEL	BP	450.9			2016CHI
$C_{10}H_{12}$	benzocyclohexane	liq	SEL	BP	480.6	0.5		1953KAR
Benzocycloalkenes								
C_9H_8	benzocyclopentene	liq	SEL	BP	455.72	0.15	BP rev	1947FEN
Alkylnapthalenes								

$C_{10}H_8$	naphthalene	sol	SEL	MP	353.4	0.3	DSC	1980KRA
		liq	SEL1	BP	491.13	0.10	EOS	1993CHI
$C_{11}H_{10}$	1-methylnaphthalene	liq	SEL	BP	517.84	0.10	VP	1955CAM
		sol	SEL1	MP	242.65	0.15	MP	1954HIP
	2-methylnaphthalene	sol	SEL	MP	307.3	0.4	MP	1958RAM
		liq	SEL1	BP	514.25	0.15	VP	1981WIE
Polycyclic Aromatics								
$C_{12}H_8$	acenaphthylene	sol	SEL	MP	366.4	1.0	MP	1965BOY
		liq	SEL1	BP	551	5	BP est	2019DIK
	biphenylene	sol	SEL	MP	384.4	0.5	MP	1974YOK
		liq	SEL1	BP	548.5	3.0	BP est	2019DIK
$C_{12}H_{10}$	acenaphthene	sol	SEL	MP	364.0	1.0	MP	1990DON
		liq	SEL1	BP	550.4	0.4	VP isoten	1923MOR
$C_{13}H_{10}$	fluorene	liq	SEL	BP	570.2	1.0	VP	1982SIV
		sol	SEL	MP	388	2	MP SLE	1989SED
$C_{14}H_{10}$	anthracene	sol	SEL	MP	489.5	0.3	MP	1988COO
		liq	SEL1	BP	614.9	0.4	VP isoten	1923MOR
	phenanthrene	sol	SEL	MP	372.7	0.3	MP	1990DON
		liq	SEL1	BP	609.00	0.06	VP ebul	1975OSB
$C_{16}H_{10}$	fluoranthene	sol	SEL	MP	381.0	0.3	MP	1973CAS
		liq	SEL1	BP	660	5	VP	1955TSY
	pyrene	sol	SEL	MP	424.3	0.6	MP	1987JUD
		liq	SEL1	BP	668	5	VP	1955TSY
$C_{18}H_{12}$	naphthacene	sol	SEL	MP	613	2	MP	1952INO
		liq	SEL1	BP	716	2	BP	1967WAK
$C_{20}H_{12}$	perylene	sol		MP	550.9	2.3	TP	2019DIK
$C_{24}H_{12}$	coronene	sol	SEL	MP	710.5	0.5	MP	1980SMI
		liq	SEL1	BP	798.2		BP rev	1989WEA

Table 2-3(4). Oxidized Hydrocarbons

Formula	Compound	Phase	SEL	trs	T_{trs}/K	unc/K	Method	Reference
Carbon Oxides								
CO_2	carbon dioxide	sol	SEL	Sub	194.686	0.003	sub rev	1996BED
CO	carbon monoxide	gas	SEL	BP	81.64	0.26	EOS	1979BRO
		sol	SEL1	TP	68.2		EOS	2006LEM
Alkanols								
CH_4O	methanol	liq	SEL	BP	337.63	0.12	EOS	1993DER
C_2H_6O	ethanol	liq	SEL	BP	351.6	0.5	EOS	2014SCH
C_3H_8O	1-propanol	liq	SEL	BP	370.3	0.2	VLE	1995HIA
	isopropanol	liq	SEL	BP	355.39	0.08	VP	1963BID
$C_4H_{10}O$	1-butanol	liq	SEL	BP	390.8	0.2	VLE	1996GON
	2-butanol	liq	SEL	BP	372.66	0.14	VP	1963BID
	isobutanol	liq	SEL	BP	380.90	0.15	VLE	1995RED
	tert-butanol	sol	SEL	MP	298.9	0.1	MP	1988KIM
		liq	SEL1	BP	355.50	0.15	VP	1963BID
$C_5H_{12}O$	1-pentanol	liq	SEL	BP	410.9	0.3	VLE	1991YOS
	2-methyl-1-butanol	liq	SEL	BP	402.14	0.17	VP ebul	2010CEN
	2-methyl-2-butanol	liq	SEL	BP	375.30	0.17	VP ebul	2010CEN
	2-pentanol	liq	SEL	BP	392.48	0.17	VP ebul	2010CEN
	3-methyl-2-butanol	liq	SEL	BP	385.03	0.17	VP ebul	2010CEN
	3-pentanol	liq	SEL	BP	388.62	0.17	VP ebul	2010CEN
	isopentanol	liq	SEL	BP	404.73	0.17	VP ebul	2010CEN
Glycols								
$C_2H_6O_2$	1,2-ethanediol	liq	SEL	BP	470.3	0.2	EOS-rev	2018LEM
$C_3H_8O_2$	1,2-propanediol	liq	SEL	BP	461.2	0.8	EOS	2021EIS
	2-methoxyethanol	liq	SEL	BP	397.54	0.15	VLE	2012RED
Sugars								
$C_3H_8O_3$	glycerin	liq	SEL	BP	563.0	1.3	BP	2019DIK
		sol	SEL1	MP	291.1	0.5	MP	1958COS
$C_6H_{10}O_5$	cellulose	sol		MP	408.2		MP	2020POD
$C_6H_{12}O_6$	alpha-D-glucose	sol	SEL	MP	421.8	0.6	MP	2004HUR
		gas	SEL1	BP	706	50	est	2019DIK
	fructose	sol	SEL	MP	376.7	0.3	MP	2004HUR
$C_{12}H_{22}O_{11}$	sucrose	sol	SEL	MP	456	4	MP	2004HUR
Phenols								
C_7H_8O	2-methylphenol	liq		BP	464.1		VP	1958BID

		sol	SEL	MP	304.14	0.10	MP	1960AND
		liq	SEL1	BP	464.14	0.10	VP rev	1949DRE2
	4-methylphenol	sol	SEL	MP	307.84	0.20	MP	1960AND
		liq	SEL1	BP	474.99	0.10	VP rev	1949DRE2
Alkyl ethers								
C_2H_6O	dimethyl ether	gas	SEL	BP	248.37	0.09	EOS	2011WU
C_3H_8O	ethyl methyl ether	gas	SEL	BP	279.7	0.5		1941IPA
$C_4H_{10}O$	diethyl ether	liq	SEL	BP	307.56	0.15	VP	1972AMB
	isopropyl methyl ether	liq	SEL	BP	303.90	0.02		1976AMB
	n-propyl methyl ether	liq	SEL	BP	311.8			1976AMB
$C_5H_{12}O$	*n*-butyl methyl ether	liq	SEL	BP	343.29	0.02	VLE	2007BOU
	tert-butyl methyl ether	liq	SEL	BP	328.20	0.15	VLE	1999MON
$C_6H_{14}O$	diisopropyl ether	liq	SEL	BP	341.6	0.3	VLE	1996RES
	di-*n*-propyl ether	liq	SEL	BP	363.25	0.04	VP	1973MEY
	isobutyl ethyl ether	liq	SEL	BP	354.2	1.0		1932NOR
Aldehydes								
CH_2O	formaldehyde	gas	SEL	BP	254.1	0.2	VP	1935SPE
C_2H_4O	acetaldehyde	gas	SEL	BP	293.56	0.15	VLE	1950COL
C_3H_6O	propanal	liq	SEL	BP	321.19	0.15	VLE	2010GAO
C_4H_8O	butanal	liq	SEL	BP	348.0	0.4	VLE	1985HSU
	isobutanal	liq	SEL	BP	337.3	0.5		1941HEA
Alkenals								
C_3H_4O	1-propenal	gas	SEL	BP	264		BP est	2021CHE
	2-propenal	liq	SEL	BP	325.4	0.3		1979MAR
Ketones								
C_3H_6O	acetone	liq	SEL	BP	329.22	0.29	EOS	2006LEM
C_4H_8O	butanone	liq	SEL	BP	352.74	0.03	VLE	1973MAT
$C_5H_{10}O$	2-pentanone	liq	SEL	BP	375.45	0.15	VLE	1973SCH
	3-pentanone	liq	SEL	BP	375.11	0.06	VP	1965COL
Carboxylic Acids								
CH_2O_2	formic acid	liq	SEL	BP	374.1	0.4	VLE	2011BAS
		sol	SEL1	MP	281.5	0.2	MP	1981KOH
$C_2H_4O_2$	acetic acid	liq	SEL	BP	391.20	0.15	VLE	1991SAY
		sol	SEL1	MP	289.5	0.1	rev	1959MCD
$C_3H_6O_2$	propanoic acid	liq	SEL	BP	414.0	0.3	VLE	1982WIS
$C_4H_8O_2$	*n*-butanoic acid	liq	SEL	BP	436.42	0.10	VP rev	1949DRE2
$C_5H_{10}O_2$	*n*-pentanoic acid	liq	SEL	BP	459.1	0.3		1964ADR
$C_6H_{12}O_2$	*n*-hexanoic acid	liq	SEL	BP	478.2	0.5		1949PAT

Alkyl Esters								
$C_2H_4O_2$	methyl formate	liq	SEL	BP	305.1	0.3	VP	1928NEL
$C_3H_6O_2$	ethyl formate	liq	SEL	BP	327.29	0.05	VLE	1998SOT
	methyl acetate	liq	SEL	BP	330.11	0.15	VLE	2016MAT
$C_4H_8O_2$	ethyl acetate	liq	SEL	BP	350.21	0.15	VP	1965POL
	methyl propanoate	liq	SEL	BP	352.75	0.25		2014RIO
$C_5H_{10}O_2$	methyl butanoate	liq	SEL	BP	375.74	0.25	VLE	2012RIO
	n-propylacetate	liq	SEL	BP	374.7	0.4		1977SVO
Alkenyl Esters								
$C_4H_6O_2$	vinyl acetate	liq	SEL	BP	345.3	0.4	VLE	1965SWA
$C_5H_8O_2$	ethyl propenoate	liq	SEL	BP	372.59	0.15	VLE	2013LOM
	methyl 2-methylpropenoate	liq	SEL	BP	369.7	0.5	VP	1956BRO
Alkanoic Anhydrides								
$C_4H_6O_3$	acetic anhydride	liq	SEL	BP	412.62	0.15		1976RAD
$C_6H_{10}O_3$	propanoic anhydride	liq	SEL	BP	440.3	1.5		1961WRI
$C_8H_{14}O_3$	butanoic anhydride	liq	SEL	BP	471.4	2.0		1921TIM2
Oxacycloalkanes								
C2H4O	oxacyclopropane	gas	SEL	BP	283.66	0.13	EOS	2015THO
C_3H_6O	methyloxacyclopropane	liq	SEL	BP	307.56	0.25	VLE	1985KOL
	oxacyclobutane	liq	SEL	BP	320.73	0.10	VP	1980OSB
C_4H_8O	oxacyclopentane	liq	SEL	BP	339.15	0.15	VLE	1998WIS
$C_5H_{10}O$	oxacyclohexane	liq	SEL	BP	361.36	0.20	VLE	2012MEJ
Oxacycloalkadienes								
C_4H_4O	oxacyclopentadiene	liq	SEL	BP	304.51	0.08	VP	1952GUT2
C_5H_6O	2-methyloxacyclopentadiene	liq	SEL	BP	338.4	0.5	VP isoten	1971EON
Oxacycloketones								
C_3H_4O	cyclopropanone	liq	SEL	BP	333	18	BP est	2019DIK
C_4H_6O	cyclobutanone	liq	SEL	BP	372.9	0.5		1972WOL
C_5H_8O	cyclopentanone	liq	SEL	BP	403.9	0.3	BP	1972WOL
$C_6H_{10}O$	cyclohexanone	liq	SEL	BP	428.57	0.04	VP	1973MEY
$C_7H_{12}O$	2-methylcyclohexanone	liq	SEL	BP	438.0	0.5	VLE	1993BUR
	3-methylcyclohexanone	liq	SEL	BP	442.7	0.5	BP	1940WHI
	4-methylcyclohexanone	liq	SEL	BP	444.6	0.5	BP	1940WHI
Dioxanes and Trioxanes								
$C_3H_6O_3$	1,3,5-trioxane	sol	SEL	MP	335.7	2.0	MP	1963LEV
		liq	SEL1	BP	387.2	0.4	VLE	1966SER
$C_4H_8O_2$	1,3-dioxane	liq	SEL	BP	378.1	0.5	BP	1967PIH
	1,4-dioxane	liq	SEL	BP	374.3	0.3	VLE	1956MCC

Furandione and D-Camphor								
$C_{10}H_{16}O$	D-camphor	sol	SEL	MP	452	10	MP	1992AND
$C_4H_2O_3$	2,5-furandione	sol	SEL	MP	325.3	0.5	MP	1983DEW
		liq	SEL1	BP	478	5	VP rev	1947STU
Aromatic Alcohols								
C_6H_6O	phenol	liq	SEL	BP	454.91	0.10	VP rev	1949DRE2
		sol	SEL1	MP	454.91	0.10	VP rev	1949DRE2
C_7H_8O	3-methylphenol	liq	SEL	BP	475.50	0.20	VLE	1989CEP2
		sol	SEL1	MP	285.37	0.20	MP	1960AND
	benzyl alcohol	liq	SEL	BP	478.5	0.3	VLE	1998SEN
Aromatic Aldehydes and Acids								
C_7H_6O	benzaldehyde	liq	SEL	BP	451.15	0.20	VLE	1981RAO
$C_7H_6O_2$	benzoic acid	sol	SEL	MP	395.50	0.04	MP	1989HAL
		liq	SEL1	BP	523.5	0.5	VP rev	1947STU

Table 2-3(5). Nitrogen-Substituted Hydrocarbons

Formula	Compound	Phase	SEL	trs	T_{trs}/K	unc/K	Method	Reference
Hydrogen Cyanides								
CHN	hydrogen cyanide	liq	SEL	BP	298.8	0.3	VP	1926SIN
Alkylamines								
CH_5N	methylamine	gas	SEL	BP	266.84	0.15	VP	1937AST
C_2H_7N	ethylamine	gas	SEL	BP	289.79	0.18	VP rev	1947STU
C_3H_9N	*n*-propylamine	liq	SEL	BP	320.38	0.06	VP ebul	1968OSB
	isopropylamine	liq	SEL	BP	304.92	0.06	VP ebul	1968OSB
$C_4H_{11}N$	isobutylamine	liq	SEL	BP	341.1	0.2		1977RAD
	n-butylamine	liq	SEL	BP	350.1	0.3	VLE	1971LET
	tert-butylamine	liq	SEL	BP	317.19	0.06	VP ebul	1968OSB
C_2H_7N	dimethylamine	gas	SEL	BP	280.02	0.15	VP	1939AST
C_3H_9N	methylethylamine	liq	SEL	BP	305.6	0.5	VLE	1985WOL
$C_4H_{11}N$	diethylamine	liq	SEL	BP	328.48	0.15		1971LET
C_3H_9N	trimethylamine	gas	SEL	BP	276.00	0.15	VP	1944AST
$C_6H_{15}N$	triethylamine	liq	SEL	BP	361.93	0.25	VLE	1962BIT
Cycloalkylamines								
$C_6H_{13}N$	cyclohexylamine	liq	SEL	BP	406.98	0.15	VLE	1960NOV
Azacycloalkanes								
C_2H_5N	azacyclopropane	liq	SEL	BP	328.6	1.0		1956SEA
C_3H_7N	azacyclobutane	liq	SEL	BP	333.5	1.5		2019DIK
C_4H_9N	azacyclopentane	liq	SEL	BP	359.71	0.15	VP	1959MCC
$C_5H_{11}N$	azacyclohexane	liq	SEL	BP	379.37	0.06	VP ebul	1968OSB
Methenamines								
$C_6H_{12}N_4$	methenamine	sol	SEL	MP	359	10	sub	2002VER
Azacycloalkadienes								
C_4H_5N	azacyclopentadiene	liq	SEL	BP	402.93	0.06	VP ebul	1968OSB
C_5H_7N	1-methylazacyclopentadiene	liq	SEL	BP	385.90	0.06	VP ebul	1968OSB
Alkanenitriles								
C_2H_3N	ethanenitrile	liq	SEL	BP	355.05	0.15	VP	1974DOJ
C_3H_5N	propanenitrile	liq	SEL	BP	370.7	0.3	VP rev	1949DRE2
C_4H_7N	butanenitrile	liq	SEL	BP	390.77	0.04	VP	1973MEY
C_5H_9N	pentanenitrile	liq	SEL	BP	414.42	0.10	VP rev	1949DRE2
$C_6H_{11}N$	hexanenitrile	liq	SEL	BP	436.61	0.04	VP	1973MEY
Alkenenitriles								

C_3H_3N	propenenitrile	liq	SEL	BP	351.1	0.5	VLE	1964SEV
Cyanogens								
C_2N_2	cyanogen	gas	SEL	BP	251.92	0.20	VP	1939RUE
Alkylhydrazines								
$C_2H_8N_2$	1,1-dimethylhydrazine	liq	SEL	BP	335.4	0.3	VLE	1992FER
Melamines								
$C_3H_6N_6$	melamine	sol	SEL	MP	627		MP	2005LID
Pyridines								
C_5H_5N	pyridine	liq	SEL	BP	388.36	0.06	eval	2019DIK
C_6H_7N	2-methylpyridine	liq	SEL	BP	402.52	0.08	VP	1963SCO
Anilines								
C_6H_7N	aniline	liq	SEL	BP	457.1	0.2	VLE	1979KUR
$C_8H_{11}N$	*N*,*N*-dimethylaniline	liq	SEL	BP	466.5	0.4	BP	1976RAD
		sol	SEL1	MP	275.7	0.3	MP	1976RAD
Oxidized Amines								
CH_4N_2O	urea	sol	SEL	MP	406.2	0.5	TP	1972ZOR
$C_6H_{15}NO_3$	triethanolamine	liq	SEL	BP	608	5	VP extrap	1959MCD
		sol	SEL1	MP	294.7	0.5	MP	1959MCD
Alkyl Nitrates and Nitroalkanes								
CH_3NO_3	methyl nitrate	liq	SEL	BP	338.0		VLE	1947LEC
$C_3H_5N_3O_9$	Nitroglycerin	sol	SEL	MP	286.7		MP	2001ONE
CN_4O_8	Tetranitromethane	liq	SEL	BP	397.9		VP	1952EDW
		sol	SEL1	MP	287.1	0.5	MP	1955TIM
CHN_3O_6	Trinitromethane	sol	SEL	MP	292	3	MP	1939LEW
CH_3NO_2	Nitromethane	liq	SEL	BP	374.34	0.08	VP	1954MCC
Isocyanates								
$C_9H_6N_2O_2$	2,4-diisocyanatotoluene	liq	SEL	BP	524.8	2.0	VP	1975FRE
		sol	SEL1	MP	293.7	1.0	MP	2020FIS
Nitro Aromatics								
$C_6H_5NO_2$	Nitrobenzene	liq	SEL	BP	483.81	0.15	VLE	1952BRO
		sol	SEL1	MP	278.89	0.20	MP	1954WIT
$C_7H_5N_3O_6$	Trinitrotoluene	sol	SEL	MP	355.1	1.0	MP	1990HUI

Table 2-3(6). Sulfur-Substituted Hydrocarbons

Formula	Compound	Phase	SEL	trs	T_{trs}/K	unc/K	Method	Reference
Alkanethiols								
CH_4S	Methanethiol	gas	SEL	BP	279.05	0.10		1960MOR
C_2H_6S	Ethanethiol	liq	SEL	BP	308.15	0.15	VP ebul	1966OSB
C_3H_8S	1-propanethiol	liq	SEL	BP	340.87	0.15	VP	1956PEN
	Isopropanethiol	liq	SEL	BP	325.71	0.15	VP ebul	1966OSB
$C_4H_{10}S$	1-butanethiol	liq	SEL	BP	371.56	0.15	VP ebul	1966OSB
	1-isobutanethiol	liq	SEL	BP	361.64	0.15	VP ebul	1966OSB
	2-butanethiol	liq	SEL	BP	358.13	0.15	VP ebul	1966OSB
$C_5H_{12}S$	1,1-dimethyl-1-propanethiol	liq	SEL	BP	372.35	0.15	BP ebul	1960HAI
				BP	372.28	0.15	VP ebul	1966OSB
	1-pentanethiol	liq	SEL	BP	399.79	0.15	VP ebul	1966OSB
	isopentanethiol	liq	SEL	BP	391.47	0.15	VP	1966OSB
	neopentanethiol	liq	SEL	BP	376.81	0.15	VP	1966OSB
	tert-pentanethiol	liq	SEL	BP	398.16	0.15	VP	1966OSB
$C_6H_{14}S$	1-hexanethiol	liq	SEL	BP	425.81	0.15	VP ebul	1966OSB
$C_7H_{16}S$	1-heptanethiol	liq	SEL	BP	450.07	0.15	VP ebul	1966OSB
Alkyl Sulfides								
CS_2	carbon disulfide	liq	SEL	BP	319.37	0.15	VP	1962WAD
$C_2H_6S_2$	dimethyl disulfide	liq	SEL	BP	382.89	0.15	VP	1950SCO
C_2H_6S	dimethyl sulfide	liq	SEL	BP	310.45	0.15	VP ebul	1942OSB
C_3H_8S	ethyl methyl sulfide	liq	SEL	BP	339.80	0.15	VP ebul	1952WHI
$C_4H_{10}S$	diethyl sulfide	liq	SEL	BP	365.25	0.15	VP ebul	1966OSB
	isopropyl methyl sulfide	liq	SEL	BP	358.0	0.2		1956HAI
	methyl propyl sulfide	liq	SEL	BP	368.69	0.15	VP	1952WHI
$C_5H_{12}S$	ethyl isopropyl sulfide	liq	SEL	BP	380.4	1.0	VP	1952WHI
	ethyl propyl sulfide	liq	SEL	BP	391.65	0.15	VP	1952WHI
$C_6H_{14}S$	di-*n*-propyl sulfide	liq	SEL	BP	415.98	0.15	VP	1952WHI
$C_8H_{18}S$	di-*n*-butyl sulfide	liq	SEL	BP	462.06	0.15	VP	1952WHI
C_2H_4S	thiacyclopropane	liq	SEL	BP	328.1	0.4	VP	1952GUT
Thiacycloalkanes								
C_3H_6S	thiacyclobutane	liq	SEL	BP	368.11	0.15	BP rev	2019DIK
C_4H_8S	thiacyclopentane	liq	SEL	BP	394.27	0.15	VP ebul	1966OSB
$C_5H_{10}S$	thiacyclohexane	liq	SEL	BP	368.11	0.15	BP rev	2019DIK
Thiacycloalkenes								
C_4H_4S	thiacyclopentadiene	liq	SEL	BP	357.31	0.15	VP	1949WAD

Aromatic Thiols								
C_6H_6S	benzenethiol	liq	SEL	BP	442.29	0.15	VP ebul	1966OSB
Alkyl Sulfoxides								
C_2H_6OS	dimethyl sulfoxide	liq	SEL	BP	463.86	0.20	VP	1972JAK
		sol	SEL1	MP	291.6	0.3	MP	1948DOU

Table 2-3(7). Fluorinated Hydrocarbons

Formula	Compound	Phase	SEL	trs	T_{trs}/K	unc/K	Method	Reference
Fluoroalkanes								
CH_3F	fluoromethane	gas	SEL	BP	194.8		EOS	2006LEM
CH_2F_2	difluoromethane	gas	SEL	BP	221.499	0.008	EOS	1997TIL
CHF_3	trifluoromethane	gas	SEL	BP	191.3		EOS	2003PEN
CF_4	tetrafluoromethane	gas	SEL	BP	145.1		EOS	1990PLA
C_2H_5F	fluoroethane	gas	SEL	BP	235.69	0.15	VP	1975VID
$C_2H_4F_2$	1,1-difluoroethane	gas	SEL	BP	249.13	0.05	EOS	1996OUT
	1,2-difluoroethane	liq	SEL	BP	304	10		1955EDG
$C_2H_3F_3$	1,1,1-trifluoroethane	gas	SEL	BP	225.91	0.04	EOS	2000LEM
			SEL	BP	278.2	1.0	BP	1936HEN
$C_2H_2F_4$	1,1,1,2-tetrafluoroethane	gas	SEL	BP	247.076	0.009	EOS	1994TIL
	1,1,2,2-tetrafluoroethane	gas	SEL	BP	253.23	0.15	VP	1991MAE
C_2HF_5	pentafluoroethane	gas	SEL	BP	225.06	0.04	EOS	2005LEM
C_2F_6	hexafluoroethane	gas	SEL	BP	195.06	0.06	EOS	2006LEM
Fluoroalkenes								
C_2H_3F	fluoroethene	gas	SEL	BP	201.7	0.5	VP rev	1947STU
$C_2H_2F_2$	1,1-difluoroethene	gas	SEL	BP	187.6	1.2	BP rev	2019DIK
	1,2-difluoroethene, (E)-	gas	SEL	BP	221	20	BP est	2019DIK
	1,2-difluoroethene, (Z)-	gas	SEL	BP	220	21	BP rev	2019DIK
C_2HF_3	trifluoroethene	gas	SEL	BP	211.7	1.5	BP	1961CRA
C_2F_4	tetrafluoroethene	gas	SEL	BP	197.51	0.25	VP	1953FUR
Chloroalkanes								
CH_3Cl	chloromethane	gas	SEL	BP	248.99	0.15	VLE	1948GAN
CH_2Cl_2	dichloromethane	liq	SEL	BP	312.92	0.15	VLE	1960MUE
$CHCl_3$	trichloromethane	liq	SEL	BP	334.42	0.18	VP rev	1947STU
CCl_4	tetrachloromethane	liq	SEL	BP	349.88	0.05	VP ebul	1959HIL
C_2H_5Cl	chloroethane	gas	SEL	BP	285.40	0.15	VP	1948GOR
$C_2H_4Cl_2$	1,1-dichloroethane	liq	SEL	BP	330.42	0.15	VP	1956LI
	1,2-dichloroethane	liq	SEL	BP	356.70	0.20	VLE	1996KRI
$C_2H_3Cl_3$	1,1,1-trichloroethane	liq	SEL	BP	347.35	0.20	BP ebul	1985RED
	1,1,2-trichloroethane	liq	SEL	BP	386.82	0.10	VP rev	1949DRE2
$C_2H_2Cl_4$	1,1,1,2-tetrachloroethane	liq	SEL	BP	403.3	0.3	VP rev	1949DRE2
	1,1,2,2-tetrachloroethane	liq	SEL	BP	422.3	1.0	VP	1950MAT
C_2HCl_5	pentachloroethane	liq	SEL	BP	435.1	0.3	VLE	1988MIH
C_2Cl_6	hexachloroethane	sol	SEL	MP	460.2	2.0	MP	1962SHA

		liq	SEL1	BP	463.0	0.5	VP rev	1947STU
Chloroalkenes								
C_2H_3Cl	chloroethene	gas	SEL	BP	259.35	0.05	VP ebul	1959MCD
$C_2H_2Cl_2$	1,1-dichloroethene	liq	SEL	BP	304.71	0.05	VP ebul	1959HIL2
	1,2-dichloroethene, (E)-	liq	SEL	BP	320.73	0.25	VP	1947KET
	1,2-dichloroethene, (Z)-	liq	SEL	BP	333.6	0.5	VP	1947KET
C_2HCl_3	trichloroethene	liq	SEL	BP	360.5	0.4	VP isoten	1944MCD
C_2Cl_4	tetrachloroethene	liq	SEL	BP	394.29	0.15	VLE	1970POL
Chloroacetylenes								
C_2HCl	chloroacetylene	gas	SEL	BP	238	10	BP rev	1987STE
C_2Cl_2	dichloroacetylene	sol	SEL	explod	306	10	explod	2021EPA
Chloroaromatics								
C_6H_5Cl	chlorobenzene	liq	SEL	BP	405.21	0.25	EOS-rev	2018LEM
Bromoalkanes								
CH_3Br	bromomethane	gas	SEL	BP	276.70	0.15	VP	1947BEE
CH_2Br_2	dibromomethane	liq	SEL	BP	370.1	0.1	VP rev	1979KUD
$CHBr_3$	tribromomethane	liq	SEL	BP	422.36	0.05	VP rev	1979KUD
CBr_4	tetrabromomethane	sol	SEL	MP	367.6	2.0	MP	1970SIL
		liq	SEL1	BP	462.6	0.6	BP rev	1979KUD
C_2H_5Br	bromoethane	liq	SEL	BP	311.54	0.19	VP	1930ZMA
$C_2H_4Br_2$	1,2-dibromoethane	liq	SEL	BP	404.56	0.10	VP rev	1949DRE
Bromoalkenes								
C_2H_3Br	bromoethene	liq	SEL	BP	306	18	BP est	2019DIK
Iodoalkanes								
CH_3I	iodomethane	liq	SEL	BP	315.58	0.02	VP rev	1979KUD
Chlorofluoromethanes								
CH_2ClF	chlorofluoromethane	gas	SEL	BP	264.1	1.0	BP rev	1979KUD
$CHClF_2$	chlorodifluoromethane	gas	SEL	BP	232.32	0.02	VP rev	1979KUD
$CHCl_2F$	dichlorofluoromethane	gas	SEL	BP	282.05	0.10	VP rev	1979KUD
$CHClF_2$	difluorochloromethane	gas	SEL	BP	232.32	0.12	VP rev	1979KUD
$CClF_3$	chlorotrifluoromethane	gas	SEL	BP	191.7	0.1	VP rev	1979KUD
CCl_2F_2	dichlorodifluoromethane	gas	SEL	BP	243.38	0.04	VP rev	1979KUD
CCl_3F	trichlorofluoromethane	gas	SEL	BP	296.78	0.02	VP rev	1979KUD
Chlorofluoroethanes								
C_2H_4ClF	1-chloro-1-fluoroethane	gas	SEL	BP	289.3	1.5	BP	1936HEN
$C_2H_3Cl_2F$	1,1-dichloro-1-fluoroethane	liq	SEL	BP	305.26	0.25	VP	1991MAE
	1,2-dichloro-1-fluoroethane	liq	SEL	BP	346.95	0.15	BP	1936HEN

$C_2H_3ClF_2$	1-chloro-1,1-difluoroethane	gas	SEL	BP	264.04	0.25	VP ebul	1993SIL
	1-chloro-2,2-difluoroethane	liq	SEL	BP	308.25	0.15	BP	1936HEN
$C_2H_2ClF_3$	2-chloro-1,1,1-trifluoroethane	gas	SEL	BP	279.25	0.15	VP	1936HEN
Chlorofluoroalkenes								
C_2HCl_2F	1,2-dichloro-1-fluoroethene	liq	SEL	BP	305.7	2.5	BP rev	2010SYN
C_2ClF_3	chlorotrifluoroethene	gas	SEL	BP	244.8	0.1	VP	1951OLI
Bromofluoroalkanes								
CH_2BrF	bromofluoromethane	gas	SEL	BP	290.7	2.0	BP rev	1979KUD
$CHBrF_2$	bromodifluoromethane	gas	SEL	BP	257.5	0.2	VP rev	1979KUD
$CHBr_2F$	dibromofluoromethane	liq	SEL	BP	337	2	BP rev	1979KUD
$CBrF_3$	bromotrifluoromethane	gas	SEL	BP	215.26	0.05	VP ebul	1959MCD
CBr_2F_2	dibromodifluoromethane	gas	SEL	BP	295.93	0.04	VP rev	1979KUD
CBr_3F	tribromofluoromethane	liq	SEL	BP	379.6	1.0	BP rev	1979KUD
Bromochloroalkanes								
CH_2BrCl	bromochloromethane	liq	SEL	BP	341.21	0.08	VP rev	1979KUD
$CHBrCl_2$	bromodichloromethane	liq	SEL	BP	363.3	0.4	BP rev	1979KUD
$CHBr_2Cl$	dibromochloromethane	liq	SEL	BP	393	2	BP rev	1979KUD
$CBrCl_3$	bromotrichloromethane	liq	SEL	BP	378.1	1.0	VP rev	1979KUD
CBr_2Cl_2	dibromodichloromethane	liq	SEL	BP	393	2	BP rev	1979KUD
CBr_3Cl	tribromochloromethane	liq	SEL	BP	433	1	BP rev	1979KUD
Bromochlorofluoroalkanes								
$CHBrClF$	bromochlorofluoromethane	liq	SEL	BP	309	2	BP rev	1979KUD
$CBrClF_2$	bromochlorodifluoromethane	gas	SEL	BP	269.14	0.04	VP rev	1979KUD
$CBrCl_2F$	bromodichlorofluoromethane	liq	SEL	BP	323	15	VP	1979KUD
CBr_2ClF	dibromochlorofluoromethane	liq	SEL	BP	353	2	BP rev	1979KUD
Carbonyl Halides								
$CHFO$	carbonyl fluoride	gas	SEL	BP	245.2	2.0	VP	1964FIS
CF_2O	carbonyl difluoride	gas	SEL	BP	188.58	0.20	VP	1968PAC
CCl_2O	phosgene	gas	SEL	BP	280.71	0.15	VP	1948GIA
Chlorophenols								
C_6HCl_5O	pentachlorophenol	liq	SEL	BP	583	3	VP	1947STU
		sol	SEL1	MP	462.8	1.0	MP	1959MCD

Table 2-3(8). Siloxanes

Formula	Compound	Phase	SEL	trs	T_{trs}/K	unc/K	Method	Reference
Siloxanes								
$C_6H_{18}OSi_2$	hexamethyldisiloxane	liq	SEL	BP	373.66	0.10	VP	1961SCO
$C_8H_{24}O_4Si_4$	octamethylcyclotetrasiloxane	liq	SEL	BP	448.9	0.6	EOS	2016THO
		sol	SEL1	MP	290.7	1.0	MP	1968MAR

Table 2-3(9). Notations for Methods

Method	Description
BP	Boiling point (unspec. method)
BP comp	BP compilation
BP ebul	BP ebulliometry method
BP est	Estimated BP
BP eval	Evaluated BP
BP rev	BP review
dec	Decomposition
DSC	Differential Scanning Calorimetry
DTA	Differential Thermal Analysis
EOS	Equation-of-State
est	Estimated
eval	Evaluated
explod	Explodes
GLC	Gas-Liquid Chromatography
MP	Melting point (unspec. method)
MP rev	MP review
MP SLE	MP Solid-Liquid Equilibrium

Method	Description
predict	Predicted
quote	Quoted value
rev	Review
sub	Sublimation (unspec. method)
sub rev	Sublimation review
sub SVE	Sublimation SVE
sub VP	Sublimation VP
sub, EOS	Sublimation EOS
TP	Triple point (unspec. method)
VLE	Vapor-Liquid Equilibrium (multicomponent)
VLE extrap	VLE extrapolation
VLE rev	VLE review
VP	Vapor pressure method
VP ebul	Ebulliometry method
VP extrap	VP extrapolation
VP isoten	VP isoteniscope method
VP rev	VP review

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3. Latent Enthalpies of Vaporization $\Delta_v H(T_b)$ and Enthalpies of Fusion $\Delta_{fus} H(T_m)$

3.1. **Overview**

In this work we compiled, evaluated, and recommended enthalpies of vaporization $\Delta_v H$ at normal boiling points T_b (P = 1 atm, 101.325 kPa) and enthalpies of fusion $\Delta_{fus} H$ for hydrocarbons, substituted hydrocarbons, and a few other compounds of chemical and engineering interest. We provide about 850 values for enthalpies of vaporization and 110 enthalpies of fusion for about 330 compounds (see Table 3-2) from over 350 source references, with selected recommended values provided in Table 3-3. The substituted hydrocarbons include different classes of oxygen-, nitrogen-, sulfur-, and halogen-substituted hydrocarbons. The enthalpies of vaporization provide here were derived from direct calorimetric determinations, change in vapor pressures of pure components and in mixtures (liquid-vapor equilibrium), and Equation-of-State (EOS) formulations. The values were taken from the literature, from the NIST Chemistry WebBook,[2021LIN] the NIST TRC Thermodata Engine (TDE)[2019DIK], and from NIST REFPROP.[2018LEM] (the latter are usually the most accurate, being based on EOS formulations). The recommended values of latent enthalpies of vaporization and fusion provided here were selected from reliable original sources (they are not weighted averages). Although this is an extensive compilation, it is not comprehensive, but we believe that there are sufficient data to make recommendations.

We provide uncertainties from the original sources where available. About 40 % of the latent enthalpies of vaporization have uncertainties of less than 1 %, about 30 % have uncertainties of (1 to 2) %, about 20 % have uncertainties of (2 to 5) %, and about 10 % have uncertainties of greater than 5 %. For compounds with large uncertainties in the enthalpies of vaporization (> 5 %), we provide several values from the literature to provide a range of values. The uncertainties “unc” in Table 3-2 are as reported. In most cases, it is not stated whether it is a standard uncertainty u (1σ) or an expanded uncertainty U (2σ). For those derived from equation-of-state (EOS) formulations (such as those in NIST REFPROP[2018LEM] or those provded in NIST TDE[2019DIK], they are expanded uncertainties U (2σ). All our recommended uncertainties are expanded uncertainties U (2σ).

In addition, we derive latent enthalpies of vaporization for many compounds where vapor pressure curves were readily available from Antoine equation parameters (*A*, *B*, *C*).[1988ANT] [1973WAG]. Here we compute enthalpies of vaporization at the normal boiling point ($\Delta_v H$) assuming the ideal gas law ($PV=nRT$) using a Clausius-Clapeyron relationship.

(3.1) $\ln(P_1/P_0) = A - (B / (T + C))$

(3.2) $n(P_1/P_0) = -\Delta_v H/R \ *(1/T_1 - 1/T_o)$

where P_0 = 1 atm (101.325 kPa) and T_0 and T_1 are two different temperatures near the normal boiling point.

More accurate latent enthalpies of vaporization can be derived considering the compressibility of a real gas – how much the gas deviates from an ideal gas where a real gas includes a compressibility factor *Z*. Including a correction for compressibility reduces the derived enthalpies of vaporization by about 4 %. Our analysis of the data indicates that this is more than twice than the median (1.1 %) and average (1.7 %) uncertainties, but on the order of the expanded uncertainties for the data set – which is about (3 to 5) %.

(3.3) $PV = Z * nRT$

(3.4) $\Delta_v H = -Z*RT * \delta\ln(P)/\delta(1/T)$

The compressibility factor needs to be computed for each compound. This can be done directly using experimental densities, using the principle of corresponding states employing critical temperatures (T_c) and critical pressures (P_C), or other methods. Here, instead, we determined an average compressibility factor for the compounds. We utilized NIST REFPROP [2018LEM] to compute the vapor-phase compressibility factors of about 40 compounds at their normal boiling points: (11) C_1 and C_2 hydrocarbons, (5) aromatic hydrocarbons, (7) C_1 to C_4 oxidized hydrocarbons, and (18) fluorinated and chlorinated C_1 and C_2 hydrocarbons. We found an average compressibility factor of 0.961 ± 0.0055 (1σ), or an uncertainty on this estimated compressibility of only about 0.6 %; this is less than the uncertainties in experimental determinations of latent enthalpies of vaporization – which are on the order of (1 to 2) % for standard uncertainty (1σ) and (3 to 5) % for expanded uncertainty (2σ). In the tables below, we utilize this average compressibility factor to derive corrected enthalpies of vaporization $\Delta_v H$ from vapor pressure curves ln(*P*) vs. (1/*T*) assuming ideal gases. We provide latent enthalpies of vaporization both assuming ideal gas $\Delta_v H$(IG), and corrected $\Delta_v H$ for the estimated compressibility factors.

Note: To estimate the latent enthalpy of vaporization of hydrogen peroxide (H_2O_2) from vapor pressure curves, we utilized the compressibility factor of 0.985 for water (H_2O) from NIST REFPROP[2018LEM] and estimated the uncertainty in the latent enthalpy of vaporization as 1 %.

We also provide enthalpies of fusion $\Delta_{fus}H$ and sublimation $\Delta_{sub}H$ for compounds with melting points above about 273 K (0 °C). These values are important for determining enthalpies of combustion which require enthalpies of melting or sublimation. Note the column heading in the table T_{trs} is the normal boiling point T_b (P = 1 atm) , the melting point T_{fus}, or the sublimation temperature T_{sub}. Correspondingly, the column heading $\Delta_{trs}H$ is the enthalpy of vaporization Δ_vH, the enthalpy of fusion $\Delta_{fus}H$, or the enthalpy of sublimation $\Delta_{sub}H$.

In Table 3-2, we provide methods, as best we could, that were used to determine the enthalpies of vaporization (and fusion or sublimation) from the publications. In some cases, they were not recorded during the compilation. Selected values are indicated by “SEL” for the compound in the standard phase, while “SEL1” and “SEL2” are values in other phases. The notation “u” in the *Selected* column indicates a very uncertain value, usually because it was estimated. Table 3-2 provides all values from the literature that we compiled, while Table 3-3 just provides the recommended values. See Table 3-1(2) for notation used for methods.

In Tables 3-2 and 3-3, the compounds are arranged first by primary and secondary chemical class and then by chemical formula.

Primary and Secondary Classes of Compounds

1. **Small Molecules**
2. **Hydrogen/Oxygen**
   a. Nitrogen/Hydrogen
   b. Nitrogen/Oxygen
   c. Sulfur/Hydrogen/Oxygen
   d. Boron/Hydrogen/Oxygen
   e. Hydrogen Halides
3. **Hydrocarbons**
   a. Carbon
   b. Alkenes
   c. Alkadienes
   d. Alkynes
   e. Alkenynes
   f. Alkadiynes
   g. Cycloalkanes
   h. Cycloalkenes
   i. Cycloalkadienes
   j. Bicycloalkanes
4. **Aromatic Hydrocarbons**
   a. Alkylbenzenes
   b. Alkenylbenzenes
   c. Benzocycloalkanes
   d. Benzocycloalkenes
   e. Alkylnapthalenes
   f. Polycyclic Aromatics
5. **Oxidized Hydrocarbons**
   a. Carbon Oxides
   b. Alkanols
   c. Glycols
   d. Sugars
   e. Phenols
   f. Alkyl ethers
   g. Aldehydes
   h. Alkenals
   i. Ketones
   j. Carboxylic Acids
   k. Alkyl Esters
   l. Alkenyl Esters
   m. Alkanoic Anhydrides
   n. Oxacycloalkanes
   o. Oxacycloalkadienes
   p. Oxacycloketones
   q. Dioxanes and Trioxanes
   r. Furandione and D-Camphor
   s. Aromatic Alcohols
   t. Aromatic Aldehydes and Acids
6. **Nitrogen-Substituted Hydrocarbons**
   a. Hydrogen Cyanides
   b. Alkylamines
   c. Cycloalkylamines
   d. Azacycloalkanes
   e. Methenamines
   f. Azacycloalkadienes
   g. Alkanenitriles
   h. Alkenenitriles
   i. Cyanogens
   j. Alkylhydrazines
   k. Melamines
   l. Pyridines
   m. Anilines
   n. Oxidized Amines
   o. Alkyl Nitrates and Nitroalkanes
   p. Isocyanates
   q. Nitro Aromatics
7. **Sulfur-Substituted Hydrocarbons**
   a. Alkanethiols
   b. Alkyl Sulfides
   c. Thiacycloalkanes
   d. Thiacycloalkenes
   e. Aromatic Thiols
   f. Alkyl Sulfoxides
8. **Halogen-Substituted Hydrocarbons**
   a. Fluoroalkanes
   b. Fluoroalkenes
   c. Chloroalkanes
   d. Chloroalkenes
   e. Chloroacetylenes
   f. Chloroaromatics
   g. Bromoalkanes
   h. Bromoalkenes
   i. Iodoalkanes
   j. Chlorofluoromethanes
   k. Chlorofluoroethanes
   l. Chlorofluoroalkenes
   m. Bromofluoroalkanes
   n. Bromochloroalkanes
   o. Bromochlorofluoroalkanes
   p. Carbonyl Halides
   q. Chlorophenols
9. **Siloxanes**

Table 3-1(1). Notation used for Tables 3-2 and 3-3 transition temperatures and enthalpies of transition

Term	Definition
Phase	phase at standard state 298.15 K and 1 bar
trs	transition
BP	boiling point
MP	melting point
SP	sublimation point
TP	triple point
SEL	selected value in the phase at standard state
SEL1	selected value in another phase 1 (not standard state)
SEL2	selected value in another phase 2 (not standard state)
$\Delta_v H$(IG)	enthalpy of vaporization (ideal gas), derived from vaporization curves
$\Delta_v H$	enthalpy of vaporization (real gas), estimated using compressibility factor Z = 0.961, see text
$\Delta_{trs} H$	transition enthalpy
Unc	uncertainty as reported
U	expanded uncertainty (2σ, 95 % confidence level)
Method	method used to determine $\Delta_{trs} H$, see Table 3-1(2)
Reference	reference provided at the end of this section

Table 3-1(2). Notation for methods used for transition temperatures and enthalpies of transition

Method	Description
BP	boiling point method (unspec.)
cal	calorimetry
DfusH	enthalpy of fusion
DsubH	enthalpy of sublimation
DvH	enthalpy of vaporization
EOS	Equation-of-State determination
est	estimated
eval	evaluated
ext	extrapolated
MP	melting point method (unspec.)
rev	review
SP	sublimation point method (unspec.)
TP	triple point method (unspec.)
VLE	Vapor-Liquid Equilibrium method (multicomponent)
VP	vapor pressure method (unspec.)

3.2. **Transition Temperatures T_{trs} and Enthalpies of Transition $\Delta_{trs}H$ (Compilation)**

This Table 3-2 contains all compiled transition temperatures and enthalpies of transition. The recommended values are provided in Table 3-3. See Table 3-1(2) for notation used for methods.

Table 3-2. Transition temperatures T_{trs} and enthalpies of transition $\Delta_{trs}H$

Formula	Compound	Phase	trs	T_{trs} (K)	SEL	$\Delta_v H$(IG) ---	$\Delta_{trs}H$ (kJ mol^{-1})	unc ---	Method	References
SMALL MOLECULES										
Hydrogen/Oxygen										
H_2	hydrogen	gas	BP	20.37	SEL		0.91	0.01	EOS	2009LEA
			BP	20.37		1.07			VP eval	2019DIK
			BP	20.37			0.91	0.01	EOS-rev	2018LEM
O_2	oxygen	gas	BP	90.19	SEL		6.82	0.01	EOS	1991STE
			BP	90.19			6.81	0.07	DvH eval	2019DIK
			BP	90.19			6.82	0.01	EOS-rev	2018LEM
H_2O	water	liq	BP	373.124	SEL		40.65	0.02	EOS	2002WAG
		sol	MP	273.15	SEL1		6.007	0.004	EOS	2006FEI
		sol	SP	273.15	SEL2		51.08	0.02	EOS-rev	2006FEI
		liq	BP	373.124			40.65	0.02	EOS-rev	2018LEM
H_2O_2	hydrogen peroxide	liq	BP	426.4	SEL	46.43	45.73	0.46	VLE	2004MAN
			MP	272.689	SEL1		12.5	0.1	DfusH	1954GIG
			MP	272.74	SEL2		52.8	5.3	DsubH est	2019DIK
			BP	426.4		46.03	45.34		VP eval	2019DIK
			BP	426.4		48.53	47.81		VP	1924MAA
Nitrogen/Hydrogen										
	nitrogen	gas	BP	77.36	SEL		5.58	0.00	EOS	2000SPA
			BP	77.36			5.58	0.07	DvH eval	2019DIK
			BP	77.36			5.58	0.00	EOS-rev	2018LEM
	ammonia	gas	BP	239.82	SEL		23.33	0.01	EOS-rev	2018LEM
			BP	239.82			23.32	0.12	DvH eval	2019DIK
Nitrogen/Oxygen										

N_2O	nitrous oxide	gas	BP	184.68	SEL		16.47	0.03	EOS	2006LEM
			BP	184.68			16.47	0.03	EOS-rev	2018LEM
Sulfur/Hydrogen/Oxygen										
H_2S	hydrogen sulfide	gas	BP	212.85	SEL	19.10	18.35	0.25	VP	1996LOP
			BP	212.85		18.68	18.0	0.6	VP	1951CLA
			BP	212.85			18.67	0.11	DvH	1936GIA
			BP	212.85			18.1	0.5	DvH eval	2019DIK
			BP	212.85		19.23	18.48		VP	1999DYK
Boron/Hydrogen										
B_2H_6	diborane	gas	BP	180.59	SEL	14.59		0.06	VP	1961DIT
			BP	180.59		14.39		0.06	VP eval	2019DIK
			BP	180.59		14.20		0.06	VP	1959PAR
Hydrogen Halides										
ClH	hydrogen chloride	gas	BP	188.173	SEL		16.18	0.08		2018LEM

HYDROCARBONS									
Carbon									
C	graphite	sol	SB	2603	SEL	712.9	0.8	VP	1948BRE
Alkanes									
CH_4	methane	gas	BP	111.67	SEL	8.20	0.06	EOS	1991SET
			BP	111.67		8.15	0.06	DvH eval	2019DIK
			BP	111.67		8.20	0.06	EOS-rev	2018LEM
C_2H_6	ethane	gas	BP	184.57	SEL	14.72	0.10	EOS	2006BUC
			BP	184.57		14.67	0.10	DvH eval	2019DIK
			BP	184.57		14.72	0.10	EOS-rev	2018LEM
			BP	184.48	15.27	14.68		VP	1926LOO
C_3H_8	propane	gas	BP	231.04	SEL	18.77	0.19	EOS	2009LEM
			BP	231.04		18.74	0.19	DvH eval	2019DIK
			BP	231.04		18.77	0.19	EOS-rev	2018LEM
			BP	231.04	19.61	18.84		VP	2004GLO
			BP	231.04	19.58	18.82		VP	1959ZIE
C_4H_{10}	isobutane	gas	BP	261.4	SEL	21.22	0.20	EOS	2006BUC
			BP	261.4		21.17	0.20	DvH eval	2019DIK
			BP	261.4		21.22	0.20	EOS-rev	2018LEM
			BP	261.41	22.25	21.38		VP	1940AST
	n-butane	gas	BP	272.66	SEL	22.42	0.24	EOS	2006BUC2
			BP	272.66		22.39	0.24	DvH eval	2019DIK
			BP	272.66		22.42	0.24	EOS-rev	2018LEM
			BP	272.77	23.14	22.24		VP	1940AST2
C_5H_{12}	isopentane	liq	BP	300.98	SEL	24.77	0.33	EOS	2006LEM
			BP	300.98		24.7	0.3	DvH eval	2019DIK
			BP	300.98		24.77	0.33	EOS-rev	2018LEM
			BP	301.0	25.95	24.94		VP	1947STU
			BP	301.0	25.98	24.97		VP	1945WIL
	neopentane	gas	BP	282.65	SEL	22.78	0.02		2006LEM
			BP	282.64		22.7	0.3	DvH eval	2019DIK
			BP	282.64	23.66	22.74	0.3	VP	1975HOP
			BP	282.65	23.95	23.02		VP	1974OSB
			BP	282.65		22.78	0.02		2018LEM
	n-pentane	liq	BP	309.21	SEL	25.81	0.11	EOS-rev	2018LEM
			BP	309.21		25.73	0.11	DvH eval	2019DIK

			BP	309.22		27.13	26.07		VP	1974OSB
C_6H_{14}	2,3-dimethylbutane	liq	BP	331.177	SEL		27.55	0.06		2018LEM
			BP	331.09			27.02	0.27	DvH eval	2019DIK
			BP	331.09		28.74	27.62		VP	1945WIL
	3-methylpentane	liq	BP	336.43	SEL	29.49	28.34	0.30	VLE	1999LOR
			BP	336.43			28.04	0.21	DvH eval	2019DIK
			BP	336.43			28.10	0.10	DvH	1949WAD2
			BP	336.43		29.61	28.45		VP	1945WIL
	isohexane	liq	BP	333.42	SEL		27.84	0.31	EOS	2006LEM
			BP	333.42			27.7	0.3	DvH eval	2019DIK
			BP	333.42		29.95	28.78		VLE	2010SAP
			BP	333.42			27.79		DvH rev	1985MAJ
			BP	333.42		29.37	28.22		VP	1945WIL
			BP	333.36			27.84	0.06		2018LEM
	neohexane	liq	BP	322.846	SEL		26.41	0.11		2018LEM
			BP	322.89			25.77	0.26	DvH eval	2019DIK
			BP	322.89		28.05	26.96		VLE	2013HYE
			BP	322.89			26.31		DvH rev	1985MAJ
			BP	322.89			26.30	0.30	DvH	1947WAD
			BP	322.89		27.71	26.62		VP	1945WIL
	n-hexane	liq	BP	341.87	SEL		28.88	0.13	EOS-rev	2018LEM
			BP	341.87			28.78	0.13	DvH eval	2019DIK
			BP	341.87		30.65	29.46		VLE	2011MEJ
			BP	341.87		31.53	30.30		VLE	2010FER
			BP	341.87		30.71	29.51		VLE	1984MIC
			BP	341.89		30.51	29.32		VP	1945WIL
C_7H_{16}	2,2,3-trimethylbutane	liq	BP	354.03	SEL		28.9	0.9	DvH eval	2019DIK
			BP	354.03		30.58	29.39		VP	1949FOR
	2,3-dimethylpentane	liq	BP	362.93	SEL		30.4	0.7	DvH eval	2019DIK
			BP	362.93		32.16	30.91		VP	1949FOR
	3,3-dimethylpentane	liq	BP	359.21	SEL		29.5	0.4	DvH eval	2019DIK
			BP	359.21		31.31	30.09		VP	1949FOR
	3-methylhexane	liq	BP	365.0	SEL		30.8	0.8	DvH eval	2019DIK
			BP	365.0		32.70	31.42		VP	1949FOR
	isoheptane	liq	BP	363.2	SEL		30.7	0.7	DvH eval	2019DIK
			BP	363.2		32.58	31.31		VP	1949FOR

	n-heptane	liq	BP	370.4	SEL		32.01	0.35	DvH	1926MAT
			BP	371.55			31.71	0.27	DvH eval	2019DIK
			BP	371.58		33.71	32.40		VP	1945WIL
C_8H_{18}	2,2,4-trimethylpentane	liq	BP	372.36	SEL		31.00	0.40	DvH	1982SVO
			BP	372.36			30.5	0.6	DvH eval	2019DIK
			BP	372.36			30.79		DvH	1985MAJ
			BP	372.36			31.00		DvH	1940PIT
			BP	372.36		32.19	30.93		VLE	2019BEN
			BP	372.39		32.61	31.34		VP	1945WIL
	2,2-dimethylhexane	liq	BP	379.77	SEL	33.57	32.26	0.50	VP	1965MCM
			BP	379.77			31.8	1.1	DvH eval	2019DIK
			BP	379.77		34.39	33.05		VP	1947STU
			BP	379.77		34.25	32.91		VP	1945WIL
	n-octane	liq	BP	398.79	SEL		34.34	0.15	DvH eval	2019DIK
			BP	398.79		37.08	35.63		VLE	2013RED
			BP	398.82		36.73	35.29		VP	1945WIL
C_9H_{20}	n-nonane	liq	BP	423.91	SEL		37.0	1.7	DvH eval	2019DIK
			BP	423.91		40.72	39.13		VLE	2018FER
			BP	423.95		39.59	38.04		VP	1949FOR
$C_{10}H_{22}$	n-decane	liq	BP	447.27	SEL		39.2	0.6	DvH eval	2019DIK
			BP	447.27		42.74	41.07		VLE	2018FER
			BP	447.27		42.32	40.67		VP	1945WIL
$C_{12}H_{26}$	n-dodecane	liq	BP	489.44	SEL		43.63	0.33		2004LEM
			MP	263.49	SEL1		36.84		MP	1954FIN
			BP	489.50		36.84	43.70	0.80	DvH	2019DIK
			BP	489.44			43.63	0.33		2018LEM
			MP	263.49			35.70		MP	2004MON
			MP	263.49			36.82		MP rev	1996DOM
$C_{16}H_{34}$	n-hexadecane	liq	BP	559.903	SEL		51.75	0.33		2018LEM
			MP	291.27	SEL1		53.36		MP	1954FIN
			BP	559.94			50.7	2.3	DvH est	2019DIK
			BP	559.94		56.48	54.28		VP	1954CAM
			MP	291.27			53.00		MP	2004MON
			MP	291.27			51.46		MP rev	1996DOM
Alkenes										
C_2H_4	ethene	gas	BP	169.38	SEL		13.53	0.04	EOS	2000SMU

			BP	169.38			13.51	0.04	DvH eval	2019DIK
			BP	169.38			13.53	0.04	EOS-rev	2018LEM
			BP	169.37		14.06	13.51		VP	1950MIC
C_3H_6	propene	gas	BP	225.53	SEL		18.47	0.26	EOS-rev	2018LEM
			BP	225.53			18.38	0.26	DvH eval	2019DIK
			BP	225.38		19.25	18.50		VP	1939POW
C_4H_8	1-butene	gas	BP	266.84	SEL		22.01	0.06		2005LEM2
			BP	266.83			21.9	0.4	DvH eval	2019DIK
			BP	267.43		22.40	21.53		VP	1928COF
			BP	266.84			22.01	0.06		2018LEM
	2-butene, (E)-	gas	BP	274.03	SEL		22.73	0.07		2005LEM2
			BP	274.01			22.73	0.20	DvH eval	2019DIK
			BP	274.01		23.86	22.93		VP	1945GUT
			BP	274.03			22.73	0.07		2018LEM
	2-butene, (Z)-	gas	BP	276.87	SEL		23.24	0.05		2005LEM2
			BP	276.87			23.21	0.13	DvH eval	2019DIK
			BP	276.87		24.31	23.36		VP	1944SCO
			BP	276.87			23.24	0.05		2018LEM
	isobutene	gas	BP	266.15	SEL		21.97	0.11		2005LEM2
			BP	266.05			21.97	0.23	DvH eval	2019DIK
			BP	266.05		22.49	21.61		VP	1940LAM
			BP	266.15			21.97	0.11		2018LEM
C_5H_{10}	1-pentene	liq	BP	303.101	SEL		25.215	0.010		2018LEM
			BP	303.12			25.1	0.5	DvH eval	2019DIK
			BP	303.12		26.44	25.41		VP	1950FOR
	2-methyl-1-butene	liq	BP	304.3	SEL		25.50	0.27	DvH eval	2019DIK
			BP	304.3		26.81	25.76		VP	1949SCO
	2-methyl-2-butene	liq	BP	311.72	SEL		26.17	0.28	DvH eval	2019DIK
			BP	311.72		27.57	26.49		VP eval	2019DIK
			BP	311.72		27.66	26.58		VP	1949SCO
	2-pentene, (E)-	liq	BP	309.51	SEL		26.00	0.22	DvH eval	2019DIK
			BP	309.51		27.41	26.34		VP	1950SCO2
	2-pentene, (Z)-	liq	BP	310.09	SEL		26.10	0.22	DvH eval	2019DIK
			BP	310.09		27.47	26.39		VP	1950SCO
	3-methyl-1-butene	gas	BP	293.21	SEL		23.97	0.26	DvH eval	2019DIK
			BP	293.21	SEL	25.28	24.29	0.25	VP	1950SCO

C_6H_{12}	1-hexene	liq	BP	336.64	SEL	29.44	28.29	0.30	VLE	2009MAR
			BP	336.64			28.22	0.25	DvH eval	2019DIK
			BP	336.64		30.12	28.95		VLE	2001SEG
			BP	336.64		29.88	28.71		VP	1950FOR
C_7H_{14}	1-heptene	liq	BP	366.71	SEL		31.20	0.26	DvH eval	2019DIK
			BP	366.71		33.64	32.33		VLE	1997SCH
			BP	366.71		33.09	31.80		VP	1950HAL
			BP	366.71		32.61	31.34		VP	1950FOR
C_8H_{16}	1-octene	liq	BP	394.43	SEL		34.5	0.4	DvH eval	2019DIK
			BP	394.43		36.60	35.17		VLE	1991KUU
			BP	394.43		36.13	34.72		VP	1950FOR
C_9H_{18}	1-nonene	liq	BP	420.02	SEL	39.03	37.51		VP	1950FOR
$C_{10}H_{20}$	1-decene	liq	BP	443.72	SEL		38.7	0.4	DvH eval	2019DIK
			BP	443.72		41.74	40.11		VP eval	2019DIK
			BP	443.72		41.77	40.14		VP	1950FOR
Alkadienes										
C_3H_4	allene	gas	BP	240.874	SEL		19.98	0.30		2018LEM
			BP	238.65			20.7	0.4	DvH eval	2019DIK
			BP	238.65		21.48	20.64		VP eval	2019DIK
			BP	238.32		20.70	19.90		VP	1947STU
			BP	238.65		20.26	19.47		VP	1930LIV
C_4H_6	1,2-butadiene	gas	BP	284.06	SEL		24.0	0.5	DvH est	2019DIK
			BP	291.94		24.70	23.74		VP eval	2019DIK
			BP	284.06			24.02		DvH rev	1985MAJ
			BP	284.06		25.30	24.31		VP ext	1947AST
			BP	291.94		25.65	24.65		VP	1947STU
	1,3-butadiene	gas	BP	268.44	SEL		22.29	0.25	DvH eval	2019DIK
			BP	268.62		23.38	22.47		VP	1933HEI2
C_5H_8	1,2-pentadiene	liq	BP	318.8	SEL		27.24	0.20	DvH eval	2019DIK
			BP	318.8		28.64	27.52		VP	1950FOR
			BP	318.8		28.43	27.32		VP	1969OSB
	1,3-pentadiene	liq	BP	314.9	SEL		26.8	1.1	DvH eval	2019DIK
			BP	315.4		28.14	27.05		VP	1947STU
	1,4-pentadiene	liq	BP	299.12	SEL		25.07	0.21	DvH eval	2019DIK
			BP	298.93		26.59	25.56		VP	1969OSB
			BP	298.9		26.63	25.59		VP	1940LAM

	2-methyl-1,3-butadiene	liq	BP	307.19	SEL		25.71	0.24	DvH eval	2019DIK
			BP	307.26		26.35	25.32		VP	1964GUB
Alkynes										
C_2H_2	acetylene	gas	BP	188.41	SEL		17.2	0.4	VP eval	2019DIK
			TP	192.0	SEL1		3.8	0.4	TP eval	2019DIK
			BP	188.41		17.06	16.39		VP ext	1956AMB
C_3H_4	propyne	gas	BP	249.8	SEL		23.5	0.5	DvH est	2019DIK
			BP	249.8		23.43	22.52		VP eval	2019DIK
			BP	249.8			21.96		DvH rev	1987STE
			BP	249.8		23.18	22.28		VP	1933HEI
			BP	249.8		23.84	22.91		VP	1967VAN
C_4H_6	1-butyne	gas	BP	281.23	SEL		24.70	0.05		2018LEM
			BP	281.18			24.95	0.17	DvH eval	2019DIK
			BP	281.18		25.92	24.91		VP	1950AST
C_5H_8	1-pentyne	liq	BP	313.51	SEL		25.4	1.1	DvH eval	2019DIK
	2-pentyne	liq	BP	329.27	SEL		25.0	1.1	DvH eval	2019DIK
C_6H_{10}	1-hexyne	liq	BP	344.53	SEL		30.0	0.4	DvH eval	2019DIK
			BP	344.53		32.02	30.77		VLE ext	2006BOU
			BP	344.53		31.73	30.49		VLE	1997BEL
	2-hexyne	liq	BP	357.59	SEL	33.52	32.21		VP eval	2019DIK
			BP	357.59		33.02	31.73		VP	1997NEG
	3-hexyne	liq	BP	354.58	SEL		31.6	0.4	DvH eval	2019DIK
			BP	354.58		32.53	31.26		VLE	1997NEG
			BP	356.34		33.49	32.18		VP	1965RON
Alkenynes										
C_4H_4	butenyne	gas	BP	279.18	SEL		23.9	0.7	DvH eval	2019DIK
			BP	278.5		25.31	24.33		VP	1947STU
C_5H_6	3-penten-1-yne	liq	BP	317.05	SEL		26.6	1.4	DvH eval	2019DIK
Alkadiynes										
C_4H_2	butadiyne	gas	BP	283.65	SEL		24.0	1.0	DvH eval	2019DIK
			BP	282.48		24.87	23.90		VP	1947STU
Cycloalkanes										
C_3H_6	cyclopropane	gas	BP	240.27	SEL		20.0	0.6	DvH eval	2019DIK
			BP	240.27		20.77	19.96		VP	1946RUE
C_4H_8	cyclobutane	gas	BP	285.64	SEL		23.7	0.4	DvH eval	2019DIK
			BP	285.64		24.87	23.90		VP	1953RAT

C_5H_{10}	cyclopentane	liq	BP	322.4	SEL		27.30	0.20	DvH	1959MCC2
			BP	322.4			27.1	0.4	DvH eval	2019DIK
			BP	322.4			27.49	0.17	DvH	1946SPI
			BP	322.41		28.41	27.30		VP	1945WIL
	methylcyclobutane	liq	BP	310.0	SEL		25.3	1.2	DvH eval	2019DIK
C_6H_{12}	cyclohexane	liq	BP	353.8649	SEL		29.99	0.15		2014ZHO
			BP	353.87			29.93	0.15	DvH eval	2019DIK
			BP	353.87		31.75	30.51		VLE	2013RED
			BP	353.87			30.00		DvH	1988DON
			BP	353.87			29.97		DvH	1985MAJ
			BP	353.87			30.10	0.15	DvH	1973SVO
			BP	353.87			33.33		DvH	1943AST
			BP	354.04		31.15	29.94		VP	1974KER
			BP	353.9		30.78	29.58		VP	1965MAR
			BP	353.93			30.06	0.13	DvH	1946SPI
			BP	353.89		31.30	30.08		VP	1945WIL
			BP	353.2			30.15		DvH	1926MAT
			BP	353.8649			29.99	0.15		2018LEM
	methylcyclopentane	liq	BP	344.96	SEL		29.07	0.10	DvH	1959MCC2
			BP	344.96			29.02	0.25	DvH eval	2019DIK
			BP	344.96		31.05	29.84		VLE	2010SAP
			BP	344.96			29.08		DvH rev	1985MAJ
			BP	344.96		30.46	29.27		VP	1945WIL
C_7H_{14}	1,1-dimethylcyclopentane	liq	BP	360.99	SEL	31.72	30.48		VP	1949FOR
	ethylcyclopentane	liq	BP	376.61	SEL	33.58	32.27		VP	1949FOR
	methylcyclohexane	liq	BP	374	SEL		31.23	na		2018LEM
			BP	374.12			31.2	0.4	DvH eval	2019DIK
			BP	374.12		33.41	32.11		VLE	2010SAP
			BP	374.12			31.27		DvH rev	1985MAJ
			BP	374.12			31.80	0.21	DvH	1946SPI
			BP	373.1			31.57		DvH	1926MAT
C_8H_{16}	isopropylcyclopentane	liq	BP	399.57	SEL	35.56	34.17		VP	1949FOR
	n-propylcyclopentane	liq	BP	404.1	SEL	36.57	35.15		VP	1949FOR
C_9H_{18}	isopropylcyclohexane	liq	BP	427.71	SEL	38.41	36.91		VP	1949FOR
	propylcyclohexane	liq	BP	429.87	SEL	38.87	37.36		VP	1949FOR
$C_{10}H_{20}$	1,3-diethylcyclohexane	liq	BP	445.7	SEL		37.5	1.2	DvH eval	2019DIK

	isobutylcyclohexane	liq	BP	444.47	SEL	40.27	38.69		VP	1949FOR
	tert-butylcyclohexane	liq	BP	444.74	SEL	39.86	38.30		VP	1949FOR
Cycloalkenes										
C_3H_4	cyclopropene	gas	BP	237.7	SEL		20.50	0.60		2019DIK
C_4H_6	cyclobutene	gas	BP	275.73	SEL		23.19	0.46		2018LEM
			BP	275.74			24.0	1.0	DvH eval	2019DIK
			BP	275.74		23.97	23.03		VP	1941HEI
C_5H_8	cyclopentene	liq	BP	317.39	SEL		26.9	0.4	DvH eval	2019DIK
	methylenecyclobutane	liq	BP	315.0	SEL		25.3	1.2	DvH eval	2019DIK
C_6H_{10}	cyclohexene	liq	BP	356.1	SEL		30.66	0.25	DvH	1973SVO
			BP	356.1			30.3	0.4	DvH eval	2019DIK
			BP	356.1			30.46		DvH	1985MAJ
			BP	356.1		31.65	30.42		VP	1973MEY
			BP	354.8			30.48		DvH	1926MAT
Cycloalkadienes										
C_5H_6	1,3-cyclopentadiene	liq	BP	314.7	SEL	25.00	24.02		VLE	1967LES
C_6H_8	1,3-cyclohexadiene	liq	BP	353.49	SEL	31.49	30.26		VP	1973MEY
Bicyclolalkanes										
$C_{10}H_{18}$	cis-decalin	liq	BP	468.93	SEL		39.9	0.4	DvH eval	2019DIK
			BP	468.93		42.12	40.48		VP	1955CAM
	trans-decalin	liq	BP	460.42	SEL		38.9	0.4	DvH eval	2019DIK
			BP	460.42		41.02	39.42		VP	1955CAM
$C_{12}H_{22}$	cyclohexylcyclohexane	liq	BP	511.1	SEL		43.86	0.28	DvH eval	2019DIK
			MP	276.80	SEL1		6.86		MP	2002CHI
			MP	277.2			6.78		MP rev	1996DOM

AROMATIC HYDROCARBONS										
Alkylbenzenes										
C_6H_6	benzene	liq	BP	353.22	SEL		30.75	0.06	EOS	2012THO
			MP	278.67	SEL1		9.87	0.01	MP	1948OLI
			BP	353.22			30.73	0.11	DvH eval	2019DIK
			BP	353.22			30.63		DvH	1990AMB
			BP	353.22			30.72		DvH rev	1985MAJ
			BP	353.22			30.75	0.06	EOS-rev	2018LEM
			BP	353.29		32.06	30.81		VP	1971EON
			BP	353.25		31.95	30.70		VP	1945WIL
			BP	353.4			30.83		DvH	1926MAT
			BP	353.22		32.14	30.89		VLE	2014NIC
			MP	278.67			9.87		MP rev	1996DOM
			MP	278.67			9.30		MP	1979SMI
			MP	278.67			9.92		MP	1942ZIE
C_7H_8	toluene	liq	BP	383.75	SEL		33.23	0.16	EOS	2006LEM
			MP	178.15	SEL1		6.64	0.01	MP	1962SCO
			BP	383.75			33.16	0.16	DvH eval	2019DIK
			BP	383.75		35.33	33.95		VLE	2020MOO
			BP	383.75			33.234	0.163	EOS-rev	2018LEM
			BP	383.77		34.80	33.44		VP	1945WIL
			BP	382.8			33.35		DvH	1926MAT
			MP	178.15			6.61		MP rev	1996DOM
			MP	178.15			6.85		MP rev	1991ACR
			MP	178.15			6.55		MP	1942ZIE
			MP	178.15			6.61		MP	1930SOU
			MP	178.15			6.62		MP	1929KEL
C_8H_{10}	1,2-dimethylbenzene	liq	BP	417.521	SEL		36.38	0.18		2012CHO
			BP	417.56			36.5	0.3	DvH eval	2019DIK
			BP	417.56		39.33	37.79		VLE	2005ROD
			BP	417.56			36.38	0.18	EOS-rev	2018LEM
			BP	417.56			36.38	0.32	EOS	2012ZHO
			BP	417.56		38.39	36.90		VP	1945WIL
			BP	414.6			36.82		DvH	1926MAT
	1,3-dimethylbenzene	liq	BP	412.214	SEL		36.11	0.07		2012CHO
			BP	412.25			36.0	0.4	DvH eval	2019DIK

			BP	412.25		38.07	36.59		VLE	2005ROD
			BP	412.25			36.11	0.40	EOS	2012ZHO
			BP	411.11		36.69	35.25		VP	1967AMB
			BP	412.25		37.93	36.45		VP	1945WIL
			BP	411.5			36.36		DvH	1926MAT
			BP	412.214			36.11	0.07	EOS-rev	2018LEM
	1,4-dimethylbenzene	liq	BP	411.47	SEL		35.71	0.07		2012CHO
			BP	411.47			35.87	0.18	DvH eval	2019DIK
			BP	411.47		38.68	37.17		VLE	2005ROD
			BP	411.47			35.71	0.20	EOS	2012ZHO
			BP	411.53		37.69	36.22		VP	1974OSB
			BP	411.11		36.69	35.25		VP	1967AMB
			BP	411.5		37.67	36.20		VP	1945WIL
			BP	410.3			35.99	0.20	DvH	1926MAT
			BP	411.47			35.71	0.07	EOS-rev	2018LEM
	ethylbenzene	liq	BP	409.314	SEL		35.60	0.11		2012ZHO
			BP	408.96			35.47	0.23	DvH eval	2019DIK
			BP	408.96		37.46	36.00		VLE	2010MAT
			BP	408.96		36.56	35.14		VP	1967AMB
			BP	409.34		37.42	35.96		VP	1945WIL
			BP	408.3			36.02	0.25	DvH	1926MAT
			BP	409.314			35.60	0.11		2018LEM
C_9H_{12}	1,2,3-trimethylbenzene	liq	BP	449.23	SEL	41.95	40.31		VP	1949FOR
	1,2,4-trimethylbenzene	liq	BP	442.5	SEL	41.29	39.68		VP	1949FOR
	1,3,5-trimethylbenzene	liq	BP	437.87	SEL	41.12	39.52		VP	1949FOR
	2-ethyltoluene	liq	BP	438.25	SEL	40.70	39.11		VP	1949FOR
	3-ethyltoluene	liq	BP	434.46	SEL	40.40	38.83		VP	1949FOR
	4-ethyltoluene	liq	BP	435.14	SEL	40.24	38.67		VP	1949FOR
	isopropylbenzene	liq	BP	425.54	SEL		37.0	0.4	DvH eval	2019DIK
			BP	425.54		39.03	37.50		VLE	1989CEP
			BP	425.54		39.03	37.51		VP	1945WIL
	n-propylbenzene	liq	BP	432.32	SEL	39.75	38.20		VP	1949FOR
$C_{10}H_{14}$	1,2-diethylbenzene	liq	BP	456.57	SEL	42.71	41.04		VP	1949FOR
	1,3-diethylbenzene	liq	BP	454.25	SEL	42.65	40.98		VP	1949FOR
	1,4-diethylbenzene	liq	BP	456.9	SEL	42.68	41.01		VP	1949FOR
	2-isopropyltoluene	liq	BP	451.5	SEL		39.3	0.7	DvH eval	2019DIK

			BP	451.45		42.69	41.02		VP	1959MCD
	3-isopropyltoluene	liq	BP	448.35	SEL		39.3	0.7	DvH eval	2019DIK
			BP	448.06		42.42	40.76		VP	1959MCD
	4-isopropyltoluene	liq	BP	450.27	SEL		39.3	0.4	DvH eval	2019DIK
			BP	450.27		41.93	40.29		VP	1959MCD
	n-butylbenzene	liq	BP	456.42	SEL	42.53	40.87		VP	1949FOR
	tert-butylbenzene	liq	BP	442.27	SEL	40.61	39.03		VP	1949FOR
Alkenylbenzenes										
C_8H_8	ethenylbenzene	liq	BP	418.45	SEL		36.8	0.4	DvH eval	2019DIK
			BP	418.45		38.83	37.32		VP	1949BUC
			BP	418.3		39.00	37.48		VP	1955DRE
Benzocycloalkanes										
$C_{10}H_{12}$	benzocyclohexane	liq	BP	480.56	SEL		42.6	0.5	DvH eval	2019DIK
			BP	480.55		44.40	42.67		VP	1922HER
Benzocycloalkenes										
C_9H_8	benzocyclopentene	liq	BP	454.72	SEL		40.36	0.4	DvH eval	2019DIK
			BP	454.72		44.77	43.02		VP	1947STU
Alkylnapthalenes										
$C_{10}H_8$	naphthalene	sol	MP	353.40	SEL		18.993	0.019	MP	2002CHI
			BP	491.11	SEL1		43.3	0.8	DvH eval	2019DIK
			SP	298.15	SEL2		72.44	0.3	VP	2005RUZ
			BP	490.73		45.79	44.01		VP	1968FOW
			BP	491.11		45.18	43.42		VP	1955CAM
			MP	353.40			19.10		MP	2008SHA
			MP	353.40			19.55		MP	2006KHI
			MP	353.40			19.10		MP rev	1991ACR
			MP	353.40			18.98	0.02	MP	1957MCC
			MP	353.40			19.00		MP	1926AND
			SP	353.37			70.38	0.3	VP	2005RUZ
			SP	298.15			73.00	0.25	VP	1972IRV
$C_{11}H_{10}$	1-methylnaphthalene	liq	BP	517.84	SEL		46.3	0.3	DvH eval	2019DIK
			MP	242.65	SEL1		6.95		MP	1957MCC
			BP	517.84		48.51	46.62		VP	1955CAM
			MP	242.65			6.95		MP rev	1996DOM
	2-methylnaphthalene	sol	MP	307.70	SEL		12.13		MP rev	1996DOM
			BP	514.2	SEL1	48.23	46.35		VP	1955CAM

			MP	307.20			11.97		MP	1931HUF
Polycyclic Aromatics										
$C_{12}H_8$	acenaphthylene	sol	MP	366.40	SEL		10.96		MP rev	1996DOM
			MP	550.60	SEL1		46.4	2.4	DvH est	2019DIK
	biphenylene	sol	MP	384.40	SEL		82.7		DsubH est	1995NAS
			BP	548.50	SEL1		46.3	1.7	DvH est	2019DIK
			MP	384.40			82.4	1.0	DsubH est	2019DIK
$C_{12}H_{10}$	acenaphthene	sol	MP	364.02	SEL		21.46		MP	1977FIN
			BP	550.39	SEL1	53.88	51.78		VP	1923MOR
			MP	364.02			21.46		MP rev	1996DOM
$C_{13}H_{10}$	fluorene	sol	MP	387.90	SEL		19.10		MP	2000LIS
			BP	570.19	SEL1	56.87	54.65		VP	1923MOR
			MP	387.90			19.58		MP rev	1996DOM
$C_{14}H_{10}$	anthracene	sol	MP	489.50	SEL		29.37		MP	1970GOU
			BP	614.87	SEL1	58.54	56.25		VP	1923MOR
			MP	489.50			29.80		MP	2003ROJ
			MP	489.50			29.37		MP rev	1996DOM
	phenanthrene	sol	MP	372.74	SEL		16.60		MP	2003ROJ
			BP	609.0	SEL1	59.56	57.24		VP	1975OSB
			BP	611.47		58.74	56.45		VP	1923MOR
			MP	372.74			16.20		MP	2000LIS
			MP	372.74			16.46		MP rev	1996DOM
			MP	372.74			15.72		MP	1992SAB
			MP	372.74			16.47		MP rev	1991ACR
$C_{16}H_{10}$	fluoranthene	sol	MP	381.00	SEL		18.73		MP	1971WON
			BP	659.82	SEL1	51.46	49.45		VP	1955TSY
			MP	381.00			18.74		MP rev	1996DOM
	pyrene	sol	MP	424.30	SEL		16.70		MP	2003ROJ
			BP	668.17	SEL1	56.54	54.34		VP	1955TSY
			MP	424.30			17.36		MP rev	1996DOM
			MP	424.30			17.11		MP rev	1991ACR
$C_{20}H_{12}$	perylene	sol	MP	550.90	SEL		32.58		MP	1992SAB
			MP	550.90			31.88		MP rev	1996DOM
			MP	550.90			31.75		MP rev	1991ACR
$C_{24}H_{12}$	coronene	sol	MP	710.50	SEL		21.20		MP	2009TOR
			MP	710.50			19.20		MP rev	1991ACR

OXIDIZED HYDROCARBONS										
Carbon Oxides										
CO_2	carbon dioxide	gas	SP	194.67	SEL		25.230	0.002	DsubH	1937GIA
			TP	216.57	SEL1		25.64	0.25	TP eval	2019DIK
CO	carbon monoxide	gas	BP	81.64	SEL		6.01	0.02	EOS	2006LEM
			BP	81.64			6.03	0.17	DvH eval	2019DIK
			BP	81.64			6.01	0.02	EOS-rev	2018LEM
Alkanols										
CH_4O	methanol	liq	BP	337.63	SEL		35.28	0.21	EOS	1993REU
			BP	337.63			35.36	0.21	DvH eval	2019DIK
			BP	337.63		38.37	36.88		VLE	2018STU
			BP	337.63			35.28	0.21	EOS-rev	2018LEM
			BP	337.7		37.31	35.85		VP	1970AMB
			BP	337.0			35.30		DvH	1926MAT
C_2H_6O	ethanol	liq	BP	351.57	SEL		39.14	0.47	EOS	2014SCH
			BP	351.57			39.1	0.5	DvH eval	2019DIK
			BP	351.57			39.14	0.47	EOS-rev	2018LEM
			BP	351.45		40.63	39.04		VP	1970AMB
			BP	351.45		40.77	39.18		VLE	1949KRE
			BP	350.6			38.91		DvH	1926MAT
C_3H_8O	1-propanol	liq	BP	370.26	SEL		41.7	0.4	DvH eval	2019DIK
			BP	370.3		43.19	41.51		VP	1970AMB
			BP	370.35		43.75	42.05		VP	1969KEM
	isopropanol	liq	BP	354.4	SEL		40.04	0.25	DvH	1926MAT
			BP	355.39			39.92	0.24	DvH eval	2019DIK
			BP	355.39		41.99	40.35		VP	1963BID
$C_4H_{10}O$	1-butanol	liq	BP	390.77	SEL		42.9	0.5	DvH eval	2019DIK
			BP	391.02		44.64	42.90		VP	1969KEM
			BP	391.36		44.93	43.18		VP	1965HES
			BP	390.88		45.04	43.29		VP	1963BID
			BP	389.9			43.82		DvH	1926MAT
	2-butanol	liq	BP	372.66	SEL	42.90	41.22		VP	1963BID
	isobutanol	liq	BP	381.04	SEL	44.01	42.29	0.40	VP	1963BID
			BP	380.9			42.0	0.3	DvH eval	2019DIK

			BP	380.0			42.87		DvH	1926MAT
	tert-butanol	sol	MP	298.87	SEL		6.78		MP	1926PAR
			BP	355.5	SEL1		39.15	0.22	DvH eval	2019DIK
			SP	298.15	SEL2		49	5	est	2022TWE
			BP	355.47		41.54	39.92		VP	1969BRO
			BP	355.49		41.54	39.92		VP	1963BEY
			BP	355.5		41.36	39.75		VP	1963BID
			MP	298.87			6.70		MP rev	1996DOM
			MP	298.87			6.79		MP rev	1991ACR
$C_5H_{12}O$	1-pentanol	liq	BP	410.9	SEL		44.2	0.6	DvH eval	2019DIK
	2-methyl-1-butanol	liq	BP	402.14	SEL		43.5	0.5	DvH eval	2019DIK
			BP	403.8		45.99	44.20		VP	1935BUT
	2-pentanol	liq	BP	392.29	SEL	44.53	42.79		VP	1935BUT
	isopentanol	liq	BP	404.73	SEL		43.6	0.3	DvH eval	2019DIK
Glycols										
$C_2H_6O_2$	1,2-ethanediol	liq	BP	470.313	SEL		54.56	na		2018LEM
			BP	470.73			52.7	1.0	DvH eval	2019DIK
			BP	470.73		54.59	52.47		VP	1952JON
$C_3H_8O_2$	1,2-propanediol	liq	BP	461.22	SEL	53.58	51.49		VP	2002STE
			BP	461.22			51.54	0.7	DvH eval	2019DIK
			BP	461.22		53.26	51.18		VP eval	2019DIK
	2-methoxyethanol	liq	BP	397.54	SEL		39.59	0.26	DvH eval	2019DIK
			BP	397.29		41.71	40.08		VP	1956PIC
Sugars										
$C_3H_8O_3$	glycerin	liq	BP	563.0	SEL		63.3	1.5	DvH eval	2019DIK
			MP	291.05	SEL1		18.29		MP	1923GIB
		sol	MP	291.05			18.28		MP rev	1991ACR
$C_6H_{12}O_6$	alpha-D-glucose	sol	MP	414	SEL		31.4		MP rev	2019DIK
		liq	BP	706	SEL1(u)		84.4	4.2	DvH est	2019DIK
		sol	SP	425	SEL2		194	5	VP	1990OJA
$C_{12}H_{22}O_{11}$	sucrose	sol	MP	424.4	SEL		32		cal	2014MAG
			SP	298.15	SEL2		94		est	2022TWE
Phenols										
C_7H_8O	2-methylphenol	sol	MP	304.20	SEL		15.82		MP	1967AND
			BP	464.14	SEL1	46.53	44.71		VP	1949DRE
			MP	304.14			15.90		MP	1998JAM

			MP	304.20			15.82		MP rev	1996DOM
			MP	304.14			14.80		MP	1990MEV
	4-methylphenol	sol	MP	307.84	SEL		12.71		MP	1967AND
			BP	474.99	SEL1	49.29	47.36		VP	1949DRE
			MP	307.84			8.58		MP	1998JAM
			MP	307.84			12.72		MP rev	1996DOM
			MP	307.84			11.80		MP	1990MEV
Alkyl Ethers										
C_2H_6O	dimethyl ether	gas	BP	248.37	SEL		21.43	0.90	EOS	2011WU
			BP	248.37			21.5	0.9	DvH eval	2019DIK
			BP	248.37			21.43	0.90	EOS-rev	2018LEM
			BP	248.34		22.28	21.41		VP	1941KEN
$C_4H_{10}O$	diethyl ether	liq	BP	307.56	SEL		26.55	0.27	EOS	2014THO
			BP	307.56			26.33	0.27	DvH eval	2019DIK
			BP	307.56			26.55	0.27	EOS-rev	2018LEM
			BP	307.1			26.69		DvH	1926MAT
			BP	307.63		27.99	26.90		VP	1922TAY
$C_6H_{14}O$	diisopropyl ether	liq	BP	341.49	SEL		28.99	0.17	DvH eval	2019DIK
			BP	341.49		31.03	29.82		VP	2007EFI
			BP	341.49		30.60	29.41		VLE	1999MON
			BP	341.49		30.86	29.65		VP	1969CID
	di-n-propyl ether	liq	BP	363.25	SEL	33.16	31.86		VP	1973MEY
			BP	359.5		33.29	31.99		VP	1969CID
Aldehydes										
CH_2O	formaldehyde	gas	BP	254.13	SEL		22.0	0.4	DvH est	2019DIK
			BP	254.13		23.30	22.39		VP ext	1935SPE
C_2H_4O	acetaldehyde	liq	BP	299.12	SEL		25.07	0.21	DvH eval	2019DIK
			BP	293.47	u	27.14	26.08		VLE	1963BUL
			BP	293.56		27.07	26.01		VLE	1950COL
C_3H_6O	propanal	liq	BP	321.19	SEL		28.3	0.4	DvH eval	2019DIK
			BP	321.19	u	32.38	31.12		VP	1951SMI
			BP	307.56			28.31		DvH rev	1985MAJ
C_4H_8O	butanal	liq	BP	347.95	SEL(u)		29.32	0.28	DvH eval	2019DIK
			BP	347.95	u	32.96	31.68		VLE	1963WOJ
			BP	348.33	u	31.34	30.11		VP	1959SEP
	isobutanal	liq	BP	337.26	SEL	30.73	29.54		VP	1959SEP

Alkenals										
C_3H_4O	2-propenal	liq	BP	325.4	SEL		29.6	0.3	DvH eval	2019DIK
			BP	325.4		30.86	29.66		VP	1979MAR
			BP	325.71		29.38	28.23		VP	1947STU
Ketones										
C_3H_6O	acetone	liq	BP	329.22	SEL		29.12	0.27	EOS	2006LEM
			BP	329.22			29.35	0.27	DvH eval	2019DIK
			BP	329.22		31.27	30.05		VLE ext	2008SON
			BP	329.22			29.12	0.27	EOS-rev	2018LEM
			BP	329.22			30.86		DvH rev	1987STE
			BP	329.42		30.91	29.70		VP	1974AMB
			BP	329.22			29.09		DvH	1957PEN
			BP	329.2			29.67		DvH	1926MAT
C_4H_8O	butanone	liq	BP	352.74	SEL		31.59	0.16	DvH eval	2019DIK
			BP	352.74		33.44	32.14		VLE	2008MAR
			BP	352.74			31.30		DvH rev	1985MAJ
			BP	352.74			31.30	0.10	DvH	1961NIC
			BP	352.63		32.84	31.56		VP	1961NIC
			BP	351.4			31.97		DvH	1926MAT
$C_5H_{10}O$	3-pentanone	liq	BP	375.11	SEL	35.31	33.93		VP	1965COL
			BP	376.41		30.97	29.76		VP	1949DRE
Carboxylic Acids										
CH_2O_2	formic acid	liq	BP	374.05	SEL		22.7	8.4	DvH est	2019DIK
			MP	281.47	SEL1		12.68		MP	1941STO
			BP	374.05			21.0		DvH	1930COO
$C_2H_4O_2$	acetic acid	liq	BP	391.2	SEL	38.67	37.16		VLE	2019LI
			MP	289.49	SEL1		11.72		MP	1982MAR
			BP	391.01		38.97	37.45		VP	1959MCD
			MP	289.49			11.72		MP rev	1996DOM
C_3H_6O	propanoic acid	liq	BP	413.99	SEL		29.91	0.7	DvH	1989JAS
			BP	413.99			29.7	1.2	DvH eval	2019DIK
			BP	413.99			30.63		DvH	1926MAT
C_4H_8O	n-butanoic acid	liq	BP	436.42	SEL		38.4	2.4	DvH eval	2019DIK
			BP	436.42			35.9	1.5	DvH	1989JAS
Alkyl Esters										
$C_2H_4O_2$	methyl formate	liq	BP	305.14	SEL		27.90	0.25	DvH	1976CIH

			BP	305.14			28.0	0.4	DvH eval	2019DIK
			BP	305.14			27.92		DvH rev	1985MAJ
			BP	304.5			28.24		DvH	1926MAT
$C_3H_6O_2$	ethyl formate	liq	BP	327.29	SEL		29.80	0.20	DvH	1976CIH
			BP	327.29			29.7	0.3	DvH eval	2019DIK
			BP	327.29			29.91		DvH rev	1985MAJ
			BP	326.5			30.13		DvH	1926MAT
$C_4H_8O_2$	ethyl acetate	liq	BP	349.2	SEL		32.30	0.30	DvH	1926MAT
			BP	350.21			32.05	0.27	DvH eval	2019DIK
			BP	350.21		33.60	32.29		VP	1965POL
Alkenyl Esters										
$C_4H_6O_2$	vinyl acetate	liq	BP	345.33	SEL		31.7	0.3	DvH eval	2019DIK
			BP	345.33		34.45	33.11		VLE	1965SWA
			BP	345.88		33.12	31.83		VP	1963CAP
$C_5H_8O_2$	ethyl propenoate	liq	BP	372.59	SEL		34.2	0.4	DvH eval	2019DIK
			BP	372.69		35.47	34.09		VP	1947STU
	methyl 2-methylpropenoate	liq	BP	369.73	SEL		34.14	0.28	DvH eval	2019DIK
			BP	369.73		38.82	37.30		VP	1956BRO
Oxacycloalkanes										
C_2H_4O	oxacyclopropane	gas	BP	283.59	SEL		25.47	0.19	EOS	2015THO
			BP	283.59			25.67	0.19	DvH eval	2019DIK
			BP	283.59			25.47	0.19	EOS-rev	2018LEM
			BP	283.59		26.49	25.46		VP	1959MCD
			BP	283.65		25.98	24.97		VLE	1950COL
C_3H_6O	methyloxacyclopropane	liq	BP	307.268			27.59	0.14	EOS-rev	2018LEM
Oxacycloalkadienes										
C_4H_4O	oxacyclopentadiene	liq	BP	304.51	SEL		27.03	0.18	DvH eval	2019DIK
			BP	304.51		28.05	26.96		VP	1952GUT
C_5H_6O	2-methyloxacyclopentadiene	liq	BP	338.39	SEL	30.86	29.66		VP	1971EON
Oxacycloketones										
C_4H_6O	cyclobutanone	liq	BP	367.79	SEL	37.15	35.70		VP	1942BEN
$C_6H_{10}O$	cyclohexanone	liq	BP	428.57	SEL	39.48	37.94		VP	1973MEY
Dioxanes and trioxanes										
$C_3H_6O_3$	1,3,5-trioxane	sol	MP	333.44	SEL		15.105	0.010	MP	1988VAN
			BP	387.2	SEL1		37.3	2.1	DvH est	2019DIK
			SP	298.15	SEL2		56.6	0.2	C	1969MAN

			MP	333.65			15.10		MP rev	1996DOM
			SP	298.15			57.06	0.37	DvH est	2019DIK
$C_4H_8O_2$	1,3-dioxane	liq	BP	378.13	SEL		34.3	2.4	DvH est	2019DIK
	1,4-dioxane	liq	BP	374.25	SEL		35.58	0.3	DvH	1963VIN
			BP	374.25			35.3	0.3	DvH eval	2019DIK
			BP	374.25			34.16		DvH rev	1985MAJ
			BP	374.44		35.79	34.39		VP	1938CRE
Furandione and D-Camphor										
$C_{10}H_{16}O$	D-camphor	sol	MP	463.38	SEL(u)		15.7		DfusH rev	1990DON
			BP	493.0	SEL1(u)		44.0	1.8	DvH est	2019DIK
			SP	298.15	SEL2		51.9	0.8	DsubHest	1977STE
			MP	451.80			5.30		MP rev	1979MJO
$C_4H_2O_3$	2,5-furandione	sol	MP	325.70	SEL		12.26		MP	1978MAR
			BP	478.33	SEL1		44.7	2.3	DvH est	2019DIK
			SP	298.15	SEL2		68.85	0.42	cal	2017SOU
			BP	478.33	u	44.05	42.33		VP	1947STU
			MP	325.70			12.26		MP rev	1996DOM
			MP	325.72			13.60		MP	1983DEW
			SP	319.0			70.72	0.42	cal	2017SOU
Aromatic Alcohols										
C_6H_6O	phenol	sol	MP	314.05	SEL		11.54		MP	1963AND
			BP	454.91	SEL1		45.47	0.23	DvH eval	2019DIK
			BP	454.91	u		48.10		DvH rev	1987STE
			BP	454.91		47.20	45.36		VP	1949DRE
			MP	314.05			11.51		MP rev	1996DOM
			MP	314.05			11.29		MP rev	1991ACR
			MP	314.05			11.51		MP	1972INO
			MP	314.05			12.13		MP	1957MAS
C_7H_8O	3-methylphenol	liq	BP	475.28	SEL		47.2	0.5	DvH eval	2019DIK
			MP	285.37	SEL1		10.67		MP	1998JAM
			BP	475.28		49.83	47.88		VP	1947GOL
			MP	285.37			10.71		MP rev	1996DOM
			MP	285.37			9.10		MP	1990MEV
			MP	285.37			10.71		MP	1967AND
	benzyl alcohol	liq	BP	477.4	SEL		50.49	1.00	DvH	1926MAT
			BP	478.5			47.3	0.8	DvH eval	2019DIK

			BP	478.45		50.39	48.42		VP	1949DRE
Aromatic Aldehydes and Acids										
C_7H_6O	benzaldehyde	liq	BP	451.15	SEL		40.9	0.3	DvH eval	2019DIK
			BP	451.68		42.38	40.73		VP	1947STU
$C_7H_6O_2$	benzoic acid	sol	MP	395.50	SEL		17.10		MP	2002ROY
			BP	523.53	SEL1		56.5	1.0	DvH eval	2019DIK
			SP	298.15	SEL2		89.25	0.42	VP	1990DAS
			BP	523.53		59.25	56.94		VP	1947STU
			MP	395.50			16.99		MP	2009BRI
			MP	395.50			17.30		MP	2003SHA
			MP	395.50			17.99		MP	1984PIT
			MP	395.50			18.00		MP	1953GIN

NITROGEN-SUBSTITUTED HYDROCARBONS										
Hydrogen Cyanides										
CHN	hydrogen cyanide	liq	BP	298.79	SEL		25.22	0.25	DvH eval	2019DIK
			BP	298.79	u	27.91			VP rev	1987STE
			BP	298.79	u	27.70			VP	1939GIA
			BP	298.79	u	27.78			VP	1926SIN
Alkyl Amines										
CH_5N	methylamine	gas	BP	266.84	SEL		25.94	0.23	DvH eval	2019DIK
			BP	266.84		26.84	25.79		VP	1937AST
C_2H_7N	ethylamine	gas	BP	289.79	SEL(u)		27.4	0.4	DvH eval	2019DIK
			BP	289.79	u	27.34	26.27		VP	1947STU
C_3H_9N	n-propylamine	liq	BP	320.38	SEL		29.58	0.20	DvH eval	2019DIK
			BP	320.38			29.55		DvH rev	1985MAJ
			BP	320.38		31.04	29.83		VLE	1983WOL
			BP	320.38		30.80	29.60		VP	1968OSB
			BP	321.71		30.37	29.19		VP	1947STU
	isopropylamine	liq	BP	304.92	SEL	29.03	27.90		VP	1968OSB
$C_4H_{11}N$	n-butylamine	liq	BP	350.12	SEL		32.03	0.27	DvH eval	2019DIK
	tert-butylamine	liq	BP	317.19	SEL	29.53	28.38		VP	1968OSB
C_2H_7N	dimethylamine	gas	BP	280.02	SEL		26.48	0.06	DvH	1939AST
			BP	280.02			26.51	0.27	DvH eval	2019DIK
			BP	280.02			26.40		DvH rev	1985MAJ
			BP	280.02		27.96	26.87		VP	1970WOL
			BP	280.02		27.11	26.05		VP	1935SIM
C_3H_9N	methylethylamine	liq	BP	305.6	SEL		28.4	0.5	DvH eval	2019DIK
	trimethylamine	gas	BP	276.0	SEL		23.00	0.22	DvH eval	2019DIK
			BP	276.0		24.17	23.23		VP	1944AST
$C_6H_{15}N$	triethylamine	liq	BP	361.93	SEL		31.3	0.4	DvH eval	2019DIK
			BP	361.93			31.01		DvH rev	1985MAJ
			BP	361.93		31.96	30.71		VP	1962BIT
Cycloalkylamines										
$C_6H_{13}N$	cyclohexylamine	liq	BP	406.98	SEL		35.8	0.6	DvH eval	2019DIK
			BP	406.98	u	38.90	37.38		VLE	2014RED
			BP	406.98	u	37.93	36.45		VP	1960NOV
Azacycloalkanes										
C_4H_9N	azacyclopentane	liq	BP	359.71	SEL	34.33	32.99		VP	1959MCC

$C_5H_{11}N$	azacyclohexane	liq	BP	379.37	SEL	35.14	33.77		VP	1968OSB
Methenamines										
$C_6H_{12}N_4$	methenamine	sol	SP	298.15	SEL		79.64	0.18	VP	2002VER
Azacycloalkadienes										
C_4H_5N	azacyclopentadiene	liq	BP	402.93	SEL	40.33	38.76		VP	1968OSB
			BP	399.47		41.60	39.98		VP	1971EON
C_5H_7N	1-methylazacyclopentadiene	liq	BP	385.9	SEL	36.82	35.38		VP	1968OSB
			BP	384.66		37.84	36.36		VP	1971EON
Alkanenitriles										
C_2H_3N	ethanenitrile	liq	BP	355.05	SEL		30.7	0.3	DvH eval	2019DIK
			BP	355.05			29.75		DvH rev	1985MAJ
			BP	355.05		32.51	31.24		VP	1974DOJ
C_3H_5N	propanenitrile	liq	BP	370.73	SEL		33.0	0.4	DvH eval	2019DIK
			BP	370.73		34.55	33.20		VLE	2013LAA
			BP	370.73		33.11	31.82		VP	1949DRE
C_4H_7N	butanenitrile	liq	BP	390.77	SEL		34.70	0.24	DvH eval	2019DIK
C_5H_9N	pentanenitrile	liq	BP	414.42	SEL	38.54	37.04		VP	1949DRE
$C_6H_{11}N$	hexanenitrile	liq	BP	436.61	SEL	41.24	39.63		VP	1973MEY
			BP	436.88		40.92	39.33		VP	1949DRE
C_3H_3N	propenenitrile	liq	BP	351.13	SEL(u)		30.7	0.7	DvH eval	2019DIK
			BP	351.13	u	34.40	33.06		VLE	2010HAI
			BP	351.13	u	34.18	32.85		VP rev	1990DAU
			BP	351.13	u	30.99	29.78		VLE	1964SEV
C_2N_2	cyanogen	gas	BP	252.0	SEL(u)		24.7	0.6	DvH eval	2019DIK
			BP	252.0	u		23.30	0.20	DvH	1939RUE
			BP	252.0	u	24.20	23.26		VP	1925PER
			BP	252.18	u	23.78	22.86		VP	1947STU
$C_2H_8N_2$	1,1-dimethylhydrazine	liq	BP	335.57	SEL		32.1	0.9	DvH eval	2019DIK
			BP	335.57		34.41	33.06		VP	1953AST
Melamines										
$C_3H_6N_6$	melamine	liq	SP	497	SEL		120	4	VP	1960HIR
			BP	639	SEL1		79	4	DvH est	2019DIK
Anilines										
C_6H_7N	2-methylpyridine	liq	BP	402.52	SEL	37.75	36.28		VP	1963SCO
	aniline	liq	BP	457.3	SEL		43.8	0.5	DvH eval	2019DIK
			BP	456.99		45.31	43.54		VP	1962HAT

$C_8H_{11}N$	N,N-dimethylaniline	liq	BP	466.47	SEL		42.7	0.8	DvH eval	2019DIK
			MP	275.65	SEL1		11.56		MP	1972AHM
			BP	466.47	u	45.79	44.01		VP	1976RAD
			BP	466.58	u	45.81	44.02		VP	1925NEL
Oxidized Amines										
CH_4N_2O	urea	sol	MP	406.5	SEL		14.79		MP	1987DEL
			SP	298.15	SEL1		95.5	0.3	VP	2006EME
			MP	406.17			14.60		MP	1999RAI
			MP	406.17			15.03		MP	1995FER
			MP	406.17			14.50		MP	1988GAM
			SP	298.15			94.6	2.0	VP	2003ZAI
$C_6H_{15}NO_3$	triethanolamine	liq	BP	623.15	SEL		82.0	2.0	VP	2004WRI
			BP	623.15			76.1	4.2	DvH est	2019DIK
Alkyl Nitrates and Nitroalkanes										
CH_3NO_3	methyl nitrate	liq	BP	338.0	SEL(u)		26.4	1.4	DvH est	2019DIK
$C_3H_5N_3O_9$	nitroglycerin	sol	MP	286.65			21.87		MP rev	1991ACR
CN_4O_8	tetranitromethane	liq	BP	397.95	SEL		40.74		DvH rev	1985MAJ
			SP	287.05	SEL1	47.40			DsubH	1941SEK
			BP	397.95	u	39.1		2.0	VP	1919MEN
			BP	397.95	u	39.56			VP	1952EDW
CH_3NO_2	nitromethane	liq	BP	373.1	SEL		34.46	0.30	DvH	1926MAT
			BP	374.34	u	37.64	36.18		VLE	1979MAR2
			BP	374.34	u	35.91	34.51		VP	1954MCC
			BP	374.34			34.73	0.24	DvH eval	2019DIK
Isocyanates										
$C_9H_6N_2O_2$	2,4-diisocyanatotoluene	liq	BP	524.83	SEL(u)		41.9	2.1	DvH est	2019DIK
			BP	524.83	u	53.84	51.74		VP	1975FRE
Nitro Aromatics										
$C_6H_5NO_2$	nitrobenzene	liq	BP	483.81	SEL		43.9	0.5	DvH eval	2019DIK
			MP	278.89	SEL1		12.12		MP	1936PAR
			BP	483.81		45.97	44.18		VLE	1952BRO
			MP	278.89			12.12		MP rev	1996DOM
$C_7H_5N_3O_6$	trinitrotoluene	sol	MP	355.1	SEL		23.43		DfusH	1993ACR
			BP	620.5	SEL1	73.69			VP	1948ROB
			SP	298.15	SEL2		113.2	1.5	VP	1979KUD
			MP	355.1			22.41		DfusH	1990HU

	MP	355.10	21.23	MP rev	1991ACR

SULFUR-SUBSTITUTED HYDROCARBONS										
Alkanethiols										
CH_4S	methanethiol	gas	BP	279.05	SEL		24.4	0.9	DvH eval	2019DIK
			BP	279.1		25.34	24.35		VP	1942RUS
C_2H_6S	ethanethiol	liq	BP	308.19	SEL		26.6	0.6	DvH eval	2019DIK
			BP	308.15		27.78	26.70		VP	1966OSB
C_3H_8S	1-propanethiol	liq	BP	340.87	SEL	30.80	29.60		VP	1956PEN
	isopropanethiol	liq	BP	325.71	SEL	29.12	27.99		VP	1966OSB
$C_4H_{10}S$	1-butanethiol	liq	BP	371.56		33.79	32.47		VP	1966OSB
	1-isobutanethiol	liq	BP	361.64	SEL	32.48	31.22		VP	1966OSB
	2-butanethiol	liq	BP	358.13	SEL	32.04	30.79		VP	1966OSB
$C_5H_{12}S$	1,1-dimethyl-1-propanethiol	liq	BP	372.28	SEL	32.95	31.66		VP	1966OSB
	1-pentanethiol	liq	BP	399.79	SEL	36.69	35.26		VP	1966OSB
$C_6H_{14}S$	1-hexanethiol	liq	BP	425.81	SEL	39.46	37.92		VP	1966OSB
$C_7H_{16}S$	1-heptanethiol	liq	BP	450.07	SEL	42.15	40.50		VP	1966OSB
Alkyl Sulfides										
CS_2	carbon disulfide	liq	BP	318.4	SEL		26.78	0.15	DvH	1926MAT
			BP	318.35			26.78	0.15	DvH eval	2019DIK
			BP	319.37		27.56	26.48		VP	1962WAD
$C_2H_6S_2$	dimethyl disulfide	liq	BP	382.89	SEL	34.98	33.61		VP	1950SCO
C_2H_6S	dimethyl sulfide	liq	BP	310.42	SEL		27.0	0.3	DvH eval	2019DIK
			BP	310.45		28.16	27.06		VP	1942OSB
C_3H_8S	ethyl methyl sulfide	liq	BP	339.8	SEL	30.78	29.58		VP	1952WHI
$C_4H_{10}S$	diethyl sulfide	liq	BP	365.25	SEL	33.26	31.97		VP	1966OSB
Thiacycloalkanes										
C_4H_8S	thiacyclopentane	liq	BP	394.27	SEL	35.94	34.53		VP	1966OSB
			BP	393.42		37.46	36.00		VP	1971EON
Thiacycloalkenes										
C_4H_4S	thiacyclopentadiene	liq	BP	357.31	SEL	32.63	31.35		VP	1949WAD
			BP	356.52		34.82	33.46		VP	1971EON
Aromatic Thiols										
C_6H_6S	benzenethiol	liq	BP	442.29	SEL	41.35	39.74		VP	1966OSB
Alkyl Sulfoxides										
C_2H_6OS	dimethyl sulfoxide	liq	BP	463.86	SEL		43.5	0.4	DvH eval	2019DIK
			MP	291.57	SEL1		14.37		MP	1970CLE
			BP	463.86		45.86	44.07		VP	1972JAK

	MP	291.57	14.37	MP rev	1996DOM

HALOGENATED HYDROCARBONS									
Fluoroalkanes									
CH_3F	fluoromethane	gas	BP	194.65	SEL		16.60	0.46	EOS	2006LEM
			BP	194.65			17.0	0.5	DvH eval	2019DIK
			BP	194.65		17.30	16.63	0.13	VLE	1997HOL
			BP	194.65		17.38	16.70		VP	1983OI
			BP	194.65		17.57	16.88		VP	1961FAR
			BP	194.65		17.40	16.72		VP	1961LI
			BP	194.65		17.36	16.68		VP	1948MIC
			BP	194.65		17.72	17.03		VP	1940GRO
			BP	194.65			16.60	0.46	EOS-rev	2018LEM
			BP	194.13		16.91	16.25		VLE	1999TAK
CH_2F_2	difluoromethane	gas	BP	221.5	SEL		19.87	0.20	EOS	1997TIL
			BP	221.5			20.24	0.20	DvH eval	2019DIK
			BP	221.5		20.70	19.89		VP	1993WEB
			BP	221.5		20.76	19.95		VP	1987KAN
			BP	221.5			19.87	0.20	EOS-rev	2018LEM
			BP	221.46		20.72	19.91		VLE	1999TAK
CHF_3	trifluoromethane	gas	BP	188.75	SEL		16.76	0.15	EOS	2003PEN
			BP	188.75			16.93	0.15	DvH eval	2019DIK
			BP	188.75			16.76	0.15	EOS-rev	2018LEM
			BP	190.98		17.56	16.88		VP	1962VAL
CF_4	tetrafluoromethane	gas	BP	145.56	SEL		11.83	0.27	EOS	1990PLA
			BP	145.56			11.84	0.27	DvH eval	2019DIK
			BP	145.56			11.83	0.27	EOS-rev	2018LEM
			BP	145.56		11.83	11.37		VP	1972REG
			BP	145.15		12.56	12.07		VP	1933MEN
C_2H_5F	fluoroethane	gas	BP	236.05	SEL		20.26	0.04	EOS	2016QI
			BP	236.05			20.32	0.19	DvH eval	2019DIK
			BP	236.05		20.80	19.99		VP	1961LI
			BP	236.05			20.26	0.04	EOS-rev	2018LEM
			BP	235.69		21.03	20.21		VP	1975VID
$C_2H_4F_2$	1,1-difluoroethane	gas	BP	249.13	SEL		21.79	0.72	EOS	1996OUT
			BP	249.13			21.8	0.7	DvH eval	2019DIK
			BP	249.13			21.791	0.715	EOS-rev	2018LEM
			BP	246.66		23.24	22.33		VP	1947STU

$C_2H_3F_3$	1,1,1-trifluoroethane	gas	BP	225.91	SEL		19.05	0.56	EOS	2000LEM
			BP	225.91			19.1	0.6	DvH eval	2019DIK
			BP	225.91		21.60	20.76		VLE	2001KUL
			BP	225.91			18.61		DvH	1996WEB
			BP	225.91			19.34		DvH	1955MEA
			BP	225.91			19.20	0.10	DvH	1944RUS
			BP	225.91			19.05	0.56	EOS-rev	2018LEM
			BP	225.85		20.05	19.26		VP	1944RUS
	1,1,2-trifluoroethane	gas	BP	276.81	SEL(u)		25.7	0.4	DvH eval	2019DIK
$C_2H_2F_4$	1,1,1,2-tetrafluoroethane	gas	BP	247.08	SEL		22.138	0.004	EOS	1994LIL
			BP	247.08			22.11	0.12	DvH eval	2019DIK
			BP	247.08			22.138	0.004	EOS-rev	2018LEM
	1,1,2,2-tetrafluoroethane	gas	BP	253.23	SEL		22.7	1.0	DvH eval	2019DIK
C_2HF_5	pentafluoroethane	gas	BP	225.06	SEL		19.70	0.22	EOS	2005LEM
			BP	225.06			19.58	0.22	DvH eval	2019DIK
			BP	225.06			19.70	0.22	EOS-rev	2018LEM
C_2F_6	hexafluoroethane	gas	BP	194.87	SEL		16.14	0.05	EOS	2006LEM
			BP	194.87			16.14	0.07	DvH eval	2019DIK
			BP	194.87			16.14	0.05	EOS-rev	2018LEM
			BP	194.87		16.96	16.30		VLE	1999TAK
Fluoroalkenes										
C_2H_3F	fluoroethene	gas	BP	201.65	SEL(u)		16.2	1.0	DvH est	2019DIK
			BP	201.65		15.69	15.08		VP	1947STU
$C_2H_2F_2$	1,1-difluoroethene	gas	BP	190.15	SEL		14.9	0.4	DvH eval	2019DIK
	1,2-difluoroethene, (E)-	gas	BP	231.15	SEL(u)		20.6	1.1	DvH est	2019DIK
	1,2-difluoroethene, (Z)-	gas	BP	253.15	SEL(u)		16.4	0.9	DvH est	2019DIK
C_2HF_3	trifluoroethene	gas	BP	211.7	SEL(u)		20.35	0.90	EOS	2016AKA
			BP	211.7			18.1	0.9	DvH est	2019DIK
			BP	211.7			20.35	0.90	EOS-rev	2018LEM
C_2F_4	tetrafluoroethene	gas	BP	197.51	SEL		16.83	0.15	DvH eval	2019DIK
			BP	197.51		17.61	16.93		VP	1953FUR
Chloroalkanes										
CH_3Cl	chloromethane	gas	BP	249.0	SEL		21.61	0.41	EOS	2014THO
			BP	249.0		22.20	21.33		VP	1961LI
			BP	249.0			21.54		DvH	1940MES
			BP	249.0			21.9	0.4	DvH eval	2019DIK

			BP	249.0			21.613	0.409	EOS-rev	2018LEM
			BP	248.99		22.20	21.34		VP	1948GAN
			BP	249.31		22.35	21.48		VP	1947BEE
CH_2Cl_2	dichloromethane	liq	BP	312.92	SEL		27.95	0.20	DvH	1976DEP
			BP	312.92			28.11	0.13	DvH eval	2019DIK
			BP	312.92		30.12	28.95		VLE	2010GAN
			BP	312.92		28.53	27.42		VLE	1994KRI
			BP	312.92		29.13	27.99	0.15	VLE	1960MUE
			BP	313.34		29.08	27.95		VP	1948GAN
			BP	313.6			27.98	0.20	DvH	1926MAT
$CHCl_3$	trichloromethane	liq	BP	333.3	SEL		29.37	0.25	DvH	1926MAT
			BP	334.42			29.2	0.4	DvH eval	2019DIK
			BP	334.42			29.24		DvH rev	1985MAJ
			BP	334.42		30.86	29.66		VLE	1999TEO
			BP	334.42		30.68	29.48		VLE	1995CHE
			BP	334.42		30.66	29.46		VP	1947STU
CCl_4	tetrachloromethane	liq	BP	348.6	SEL		29.96	0.40	DvH	1926MAT
			BP	349.65			29.6	0.5	DvH eval	2019DIK
			BP	349.65			29.82		DvH rev	1985MAJ
			BP	349.88		30.95	29.75		VP	1959HIL2
C_2H_5Cl	chloroethane	gas	BP	285.4	SEL		24.42	0.14	DvH eval	2019DIK
			BP	285.4		25.50	24.51		VP	1961LI
			BP	285.4		25.58	24.58		VP	1948GOR
$C_2H_4Cl_2$	1,1-dichloroethane	liq	BP	330.42	SEL		29.02	0.16	DvH eval	2019DIK
			BP	330.42		30.45	29.26		VLE	1999IGO
			BP	330.42			28.85		DvH rev	1985MAJ
			BP	330.42		30.17	28.99		VP	1956LI
	1,2-dichloroethane	liq	BP	356.7	SEL		32.090	0.032	EOS	2017THO
			BP	356.7			31.9	0.4	DvH eval	2019DIK
			BP	356.7			31.98		DvH rev	1985MAJ
			BP	356.7		32.38	31.12		VLE	1973JAG
			BP	356.7			32.090	0.032	EOS-rev	2018LEM
			BP	356.98		33.62	32.31		VP	1929PEA
$C_2H_3Cl_3$	1,1,1-trichloroethane	liq	BP	347.22	SEL(u)		29.69	0.20	DvH eval	2019DIK
			BP	347.22			29.86		DvH rev	1985MAJ
			BP	347.22		32.40	31.14		VLE	1977RAO

			BP	340.96		34.82	33.46		VP	1944RUB
	1,1,2-trichloroethane	liq	BP	386.78	SEL		34.94	0.23	DvH eval	2019DIK
			BP	386.78		38.11	36.63		VLE	1946TRE
			BP	386.82		36.11	34.70		VP	1949DRE
$C_2H_2Cl_4$	1,1,1,2-tetrachloroethane	liq	BP	403.33	SEL		35.07	0.27	DvH eval	2019DIK
			BP	403.33		37.33	35.87		VP	1949DRE
	1,1,2,2-tetrachloroethane	liq	BP	419.25	SEL(u)		38.0	0.8	DvH eval	2019DIK
			BP	419.25		38.17	36.69		DvH	1978SUN
			BP	422.32		36.66	35.23		VP	1950MAT
			BP	418.2			38.64		DvH	1926MAT
C_2HCl_5	pentachloroethane	liq	BP	433.45	SEL(u)		37.4	1.8	DvH est	2019DIK
			BP	433.45		37.40	35.94		VP rev	1943MCG
			BP	433.45		37.92	36.44		VP	1930NEL
C_2Cl_6	hexachloroethane	sol	MP	458.15	SEL		9.75		MP rev	1996DOM
			BP	458.2	SEL1(u)		37.5	1.5	DvH est	2019DIK
			SP	439	SEL2		59.0	0.8	VP	1947IVI
			BP	462.96		44.60	42.87		VP	1947STU
Chloroalkenes										
C_2H_3Cl	chloroethene	gas	BP	259.443	SEL		22.31	0.07		2018LEM
			BP	259.35		22.97	22.07		VP	1949DRE
			BP	259.35			20.4	1.0	DvH eval	2019DIK
			BP	259.35		22.85	21.96		VP	1959MCD
$C_2H_2Cl_2$	1,1-dichloroethene	liq	BP	304.71	SEL		26.46	0.26	DvH eval	2019DIK
			BP	304.71			26.14		DvH rev	1985MAJ
			BP	304.71		26.84	25.79		VP	1959HIL
			BP	304.71		27.07	26.02		VP	1959MCD
	1,2-dichloroethene, (E)-	liq	BP	320.73	SEL		27.9	0.4	DvH eval	2019DIK
			BP	320.73		29.07	27.94		VLE	1985MAC
			BP	320.73		28.67	27.55		VP	1947KET
			BP	320.73		29.89	28.7	0.5	VP	1943MCG
	1,2-dichloroethene, (Z)-	liq	BP	333.58	SEL		29.62	0.29	DvH eval	2019DIK
			BP	333.58		30.22	29.04		VP	1947KET
C_2HCl_3	trichloroethene	liq	BP	358.8	SEL		31.47	0.25	DvH	1926MAT
			BP	360.5			31.23	0.28	DvH eval	2019DIK
			BP	360.5		32.13	30.88		VP	1944MCD
C_2Cl_4	tetrachloroethene	liq	BP	394.29	SEL		34.41	0.24	DvH eval	2019DIK

			BP	394.29			34.68		DvH	1985MAJ
			BP	394.29		34.32	32.98		VLE	1996DEJ
			BP	394.29		36.23	34.82		VP	1972BOU
			BP	394.29		36.00	34.60		VLE	1970POL
Chloroaromatics										
C_6H_5Cl	chlorobenzene	liq	BP	405.21	SEL		35.53	0.44	EOS-rev	2018LEM
			BP	405.21		37.49	36.03		VLE	1989RAM
			BP	405.21		36.92	35.48		VLE	1973MOR
			BP	405.21		36.89	35.45		VLE	1952BRO
Bromoalkanes										
CH_3Br	bromomethane	gas	BP	276.7	SEL		23.5	0.5	DvH eval	2019DIK
			BP	276.7			23.9	0.3	DvH rev	1985MAJ
			BP	276.7		24.70	23.74		Vp	1961LI
			BP	276.7		24.90	23.93		VP	1947BEE
			BP	276.7		24.81	23.84		VP	1938EGA
			BP	276.7		24.96	23.98		VP	1931HIS
CH_2Br_2	dibromomethane	liq	BP	370.1	SEL		33.4	0.4	DvH eval	2019DIK
			BP	370.1		35.83	34.43		VLE ext	1973PHI
			BP	371.67		34.82	33.46		VP	1947STU
$CHBr_3$	tribromomethane	liq	BP	422.36	SEL		37.5	0.3	DvH eval	2019DIK
			BP	422.36	u		39.66		DvH rev	1985MAJ
			BP	422.36		39.53	37.98		VP ext	1972BOU
			BP	421.83		38.20	36.71		VLE	1941SIM
CBr_4	tetrabromomethane	sol	MP	367.60	SEL		3.95		MP rev	1996DOM
			BP	462.55	SEL1	40.95	39.35		VP	1947STU
			SP	298.15	SEL2		54.5	0.7	cal	1984BIC
C_2H_5Br	bromoethane	liq	BP	311.54	SEL		26.9	0.3	DvH eval	2019DIK
			BP	311.54		27.80	26.72		VP	1961LI
			BP	311.54		27.94	26.85		VP	1930ZMA
Bromoalkenes										
C_2H_3Br	bromoethene	liq	BP	311.54	SEL(u)		27.3	1.9	DvH est	2019DIK
			BP	288.6		24.89	23.92		VP	1937GUY
Chlorofluoromethanes										
CH_2ClF	chlorofluoromethane	gas	BP	264.0	SEL(u)		19.7	1.1	DvH est	2019DIK
$CHClF_2$	chlorodifluoromethane	gas	BP	232.35	SEL		20.21	0.19	EOS	1995KAM
			BP	232.35			20.21	0.19	DvH eval	2019DIK

			BP	232.35			20.21	0.19	EOS-rev	2018LEM
			BP	232.28		20.95	20.14		VP	1964KLE
$CHCl_2F$	dichlorofluoromethane	gas	BP	282.05	SEL		24.64	0.20	EOS	1990PLA
			BP	276.7			25.21		EOS	1969ALT
			BP	282.27		25.52	24.52		VP	1947STU
			BP	282.05			25.3	0.5	DvH eval	2019DIK
			BP	282.05			24.64	0.20	EOS-rev	2018LEM
			BP	276.7		25.56	24.56		VP	1940BEN
$CClF_3$	chlorotrifluoromethane	gas	BP	191.75	SEL		15.601	0.016	EOS	2000MAG
			BP	191.75		16.44	15.80		VP rev	1987STE
			BP	191.75		16.24	15.61	0.23	VP	1985FER
			BP	191.75		16.34	15.70		VP	1952ALB
			BP	191.75		15.99	15.36		VP	1933THO
			BP	191.75			15.61	0.02	DvH eval	2019DIK
			BP	191.75			15.601	0.200	EOS-rev	2018LEM
			BP	191.91		16.26	15.63		VP	1947STU
CCl_2F_2	dichlorodifluoromethane	gas	BP	243.35	SEL		20.09	0.04	EOS	1992MAR
			BP	243.35			20.08	0.22	DvH eval	2019DIK
			BP	243.35			20.09	0.04	EOS-rev	2018LEM
			BP	243.35		21.05	20.23		VP	1992HAE
			BP	243.29		20.98	20.16		VP	1947STU
CCl_3F	trichlorofluoromethane	gas	BP	296.858	SEL		24.91	0.05	EOS	2000JAC
			BP	296.95			24.85	0.16	DvH eval	2019DIK
			BP	296.858			24.91	0.05	EOS-rev	2018LEM
			BP	296.78		25.94	24.93		VP	1941OSB
			BP	296.86		25.99	24.97		VP	1940BEN
C_2ClF_3	chlorotrifluoroethene	gas	BP	244.8	SEL		20.71	0.25	DvH eval	2019DIK
			BP	244.8		21.77	20.93		VP	1951OLI
Bromofluoroalkanes										
CH_2BrF	bromofluoromethane	liq	BP	310.0	SEL(u)		30.6	1.6	DvH est	2019DIK
$CHBrF_2$	bromodifluoromethane	gas	BP	258.65	SEL		22.5	1.0	DvH eval	2019DIK
			BP	258.65		23.95	23.01		VP	1992SAL
$CBrF_3$	bromotrifluoromethane	gas	BP	215.35	SEL		17.48	0.17	DvH eval	2019DIK
			BP	215.26		18.27	17.56		VP	1959MCD
CBr_2F_2	dibromodifluoromethane	gas	BP	297.65	SEL		24.45	0.19	DvH eval	2019DIK
			BP	295.94		25.53	24.53		VP	1959MCD

CBr_3F	tribromofluoromethane	liq	BP	379.65	SEL(u)		42.6	2.1	DvH est	2019DIK
Bromochloroalkanes										
CH_2BrCl	bromochloromethane	liq	BP	341.21	SEL		30.55	0.18	DvH eval	2019DIK
			BP	341.21		31.84	30.60		VP	1959MCD
$CHBrCl_2$	bromodichloromethane	liq	BP	362.65	SEL(u)		31.8	1.7	DvH est	2019DIK
$CHBr_2Cl$	dibromochloromethane	liq	BP	393.0	SEL(u)		38.4	1.9	DvH est	2019DIK
$CBrCl_3$	bromotrichloromethane	liq	BP	376.65	SEL(u)		32.1	1.4	DvH est	2019DIK
CBr_2Cl_2	dibromodichloromethane	liq	BP	423.35	SEL(u)		34.1	1.8	DvH est	2019DIK
Bromochlorofluoroalkanes										
CHBrClF	bromochlorofluoromethane	liq	BP	312.6	SEL(u)		26.9	1.4	DvH est	2019DIK
$CBrClF_2$	bromochlorodifluoromethane	gas	BP	270.65	SEL		22.15	0.10	DvH eval	2019DIK
			BP	269.19		23.21	22.31		VP	1960GLE
$CBrCl_2F$	bromodichlorofluoromethane	liq	BP	325.15	SEL(u)		29.5	1.6	DvH est	2019DIK
CBr_2ClF	dibromochlorofluoromethane	liq	BP	352.65	SEL(u)		32.9	1.7	DvH est	2019DIK
Carbonyl Halides										
CF_2O	carbonyl difluoride	gas	BP	188.58	SEL	18.92			VP	1968PAC
CCl_2O	phosgene	gas	BP	280.71	SEL		24.40	0.05	DvH	1948GIA
			BP	280.71			24.51		DvH est	1987STE
			BP	280.71			24.4	0.5	DvH eval	2019DIK
Chlorophenols										
C_6HCl_5O	pentachlorophenol	sol	MP	462.80	SEL		17.15		MP rev	1991ACR
			BP	582.5	SEL1(u)		59.1	2.8	DvH est	2019DIK
			SP	298.15	SEL2		91.64	0.22	VP	2007VER
			SP	403.2			88.4	0.3	VP	2007VER
			BP	582.5		60.73	58.36		VP eval	2019DIK
			BP	582.5			72.81		DvH rev	1947STU

Siloxanes									
$C_6H_{18}OSi_2$	hexamethyldisiloxane	liq	BP	373.66	SEL(u)		31.32	DvH	2011ABB
			BP	373.66		33.89		VP	2011ABB
			BP	373.66		33.70		VP	1961SCO
$C_8H_{24}O_4Si_4$	octamethylcyclotetrasiloxane	liq	BP	448.02	SEL(u)		38.4 1.2	DvH eval	2019DIK
			MP	290.65	SEL1		23.77	MP rev	1996DOM
			BP	448.02		42.54		VP eval	2019DIK
			BP	448.02		42.91		VP	2011ABB
			BP	448.02		43.46		VP ext	1954OST

3.3. Recommended Transition Temperatures T_{trs} and Enthalpies of Transition $\Delta_{trs}H$

3.3.1. Data Tables for Recommended Enthalpies of Transition

These are the recommended transition temperatures and enthalpies of transition. All compiled values are provided in Table 3-2. A discussion of uncertainties in enthalpies of vaporization follows in Section 3.3.2. See Table 3-1(2) for notation used for methods.

Table 3-3. Recommended transition temperatures T_{trs} and enthalpies of transition $\Delta_{trs}H$
This table is divided into sub-tables by compound class.

Table 3-3(1). Small Molecules

Formula	Compound	Phase	trs	T_{trs} (K)	SEL	$\Delta_v H$(IG) ---	$\Delta_{trs}H$ (kJ mol^{-1})	U ---	Method	Reference
Hydrogen/Oxygen										
H_2	hydrogen	gas	BP	20.37	SEL		0.91	0.01	EOS	2009LEA
O_2	oxygen	gas	BP	90.19	SEL		6.82	0.01	EOS	1991STE
H_2O	water	liq	BP	373.124	SEL		40.65	0.02	EOS	2002WAG
		sol	MP	273.15	SEL1		6.007	0.004	EOS	2006FEI
		sol	SP	273.15	SEL2		51.08	0.02	EOS	2006FEI
H_2O_2	hydrogen peroxide	liq	BP	426.4	SEL	46.43	45.73	0.46	VLE	2004MAN
		sol	MP	272.689	SEL1		12.5	0.1	DfusH	1954GIG
		sol	MP	272.74	SEL2		52.8	5.3	DsubH est	2019DIK
Nitrogen/Hydrogen/Oxygen										
N_2	nitrogen	gas	BP	77.36	SEL		5.58	0.00	EOS	2000SPA
H_3N	ammonia	gas	BP	239.82	SEL		23.33	0.01	EOS-rev	2018LEM
N_2O	nitrous oxide	gas	BP	184.68	SEL		16.47	0.03	EOS	2006LEM
Sulfur/Hydrogen/Oxygen										
H_2S	hydrogen sulfide	gas	BP	212.85	SEL	19.10	18.35	0.25	VP	1996LOP
Boron/Hydrogen										
B_2H_6	diborane	gas	BP	180.59	SEL	14.59		0.06	VP	1961DIT
Hydrogen Halides										
ClH	hydrogen chloride	gas	BP	188.173	SEL		16.18	0.08	EOS	2018LEM

Table 3-3(2). Hydrocarbons

Formula	Compound	Phase	trs	T_{trs} (K)	SEL	$\Delta_v H$(IG) ---	$\Delta_{trs} H$ (kJ mol^{-1})	unc ---	Method	Reference
Carbon										
C	graphite	sol	SB	2603	SEL		712.9	0.8	VP	1948BRE
Alkanes										
CH_4	methane	gas	BP	111.67	SEL		8.20	0.06	EOS	1991LEM
C_2H_6	ethane	gas	BP	184.57	SEL		14.72	0.10	EOS	2006BUC
C_3H_8	propane	gas	BP	231.04	SEL		18.77	0.19	EOS	2009LEM
C_4H_{10}	isobutane	gas	BP	261.4	SEL		21.22	0.20	EOS	2006BUC
	n-butane	gas	BP	272.66	SEL		22.42	0.24	EOS	2006BUC2
C_5H_{12}	isopentane	liq	BP	300.98	SEL		24.77	0.33	EOS	2006LEM
	neopentane	gas	BP	282.65	SEL		22.78	0.02	EOS	2016LEM
	n-pentane	liq	BP	309.21	SEL		25.81	0.11	EOS-rev	2018LEM
C_6H_{14}	2,3-dimethylbutane	liq	BP	331.177	SEL		27.55	0.06	EOS	2018LEM
	3-methylpentane	liq	BP	336.43	SEL	29.49	28.34	0.30	VLE	1999LOR
	isohexane	liq	BP	333.42	SEL		27.84	0.31	EOS	2006LEM
	neohexane	liq	BP	322.846	SEL		26.41	0.11	EOS	2018LEM
	n-hexane	liq	BP	341.87	SEL		28.88	0.13	EOS-rev	2018LEM
C_7H_{16}	2,2,3-trimethylbutane	liq	BP	354.03	SEL		28.9	0.9	DvH eval	2019DIK
	2,3-dimethylpentane	liq	BP	362.93	SEL		30.4	0.7	DvH eval	2019DIK
	3,3-dimethylpentane	liq	BP	359.21	SEL		29.5	0.4	DvH eval	2019DIK
	3-methylhexane	liq	BP	365.0	SEL		30.8	0.8	DvH eval	2019DIK
	isoheptane	liq	BP	363.2	SEL		30.7	0.7	DvH eval	2019DIK
	n-heptane	liq	BP	370.4	SEL		32.01	0.35	DvH	1926MAT
C_8H_{18}	2,2,4-trimethylpentane	liq	BP	372.36	SEL		31.00	0.40	DvH	1982SVO
	2,2-dimethylhexane	liq	BP	379.77	SEL	33.57	32.26	0.50	VP	1965MCM
	n-octane	liq	BP	398.79	SEL		34.34	0.15	DvH eval	2019DIK
C_9H_{20}	n-nonane	liq	BP	423.91	SEL		37.0	1.7	DvH eval	2019DIK
$C_{10}H_{22}$	n-decane	liq	BP	447.27	SEL		39.2	0.6	DvH eval	2019DIK
$C_{12}H_{26}$	n-dodecane	liq	BP	489.44	SEL		43.63	0.33		2004LEM
		sol	MP	263.49	SEL1		36.84		MP	1954FIN
$C_{16}H_{34}$	n-hexadecane	liq	BP	559.903	SEL		51.75	0.33		2018LEM

		sol	MP	291.27	SEL1		53.36		MP	1954FIN
Alkenes										
C_2H_4	ethene	gas	BP	169.38	SEL		13.53	0.04	EOS	2000SMU
C_3H_6	propene	gas	BP	225.53	SEL		18.47	0.26	EOS-rev	2018LEM
C_4H_8	1-butene	gas	BP	266.84	SEL		22.01	0.06		2005LEM2
	2-butene, €-	gas	BP	274.03	SEL		22.73	0.07		2005LEM2
	2-butene, (Z)-	gas	BP	276.87	SEL		23.24	0.05		2005LEM2
	isobutene	gas	BP	266.15	SEL		21.97	0.11		2005LEM2
C_5H_{10}	1-pentene	liq	BP	303.101	SEL		25.215	0.010		2018LEM
	2-methyl-1-butene	liq	BP	304.3	SEL		25.50	0.27	DvH eval	2019DIK
	2-methyl-2-butene	liq	BP	311.72	SEL		26.17	0.28	DvH eval	2019DIK
	2-pentene, €-	liq	BP	309.51	SEL		26.00	0.22	DvH eval	2019DIK
	2-pentene, (Z)-	liq	BP	310.09	SEL		26.10	0.22	DvH eval	2019DIK
	3-methyl-1-butene	gas	BP	293.21	SEL	25.28	24.29	0.25	VP	1950SCO
C_6H_{12}	1-hexene	liq	BP	336.64	SEL	29.44	28.29	0.30	VLE	2009MAR
C_7H_{14}	1-heptene	liq	BP	366.71	SEL		31.20	0.26	DvH eval	2019DIK
C_8H_{16}	1-octene	liq	BP	394.43	SEL		34.5	0.4	DvH eval	2019DIK
C_9H_{18}	1-nonene	liq	BP	420.02	SEL	39.03	37.51		VP	1950FOR
$C_{10}H_{20}$	1-decene	liq	BP	443.72	SEL		38.7	0.4	DvH eval	2019DIK
Alkadienes										
C_3H_4	allene	gas	BP	240.874	SEL		19.98	0.30		2018LEM
C_4H_6	1,2-butadiene	gas	BP	284.06	SEL		24.0	0.5	DvH est	2019DIK
	1,3-butadiene	gas	BP	268.44	SEL		22.29	0.25	DvH eval	2019DIK
C_5H_8	1,2-pentadiene	liq	BP	318.8	SEL		27.24	0.20	DvH eval	2019DIK
	1,3-pentadiene	liq	BP	314.9	SEL		26.8	1.1	DvH eval	2019DIK
	1,4-pentadiene	liq	BP	299.12	SEL		25.07	0.21	DvH eval	2019DIK
	2-methyl-1,3-butadiene	liq	BP	307.19	SEL		25.71	0.24	DvH eval	2019DIK
Alkynes										
C_2H_2	acetylene	gas	BP	188.41	SEL		17.2	0.4	VP eval	2019DIK
		sol	TP	192.0	SEL1		3.8	0.4	TP eval	2019DIK
C_3H_4	propyne	gas	BP	249.8	SEL		23.5	0.5	DvH est	2019DIK
C_4H_6	1-butyne	gas	BP	281.23	SEL		24.70	0.05		2018LEM
C_5H_8	1-pentyne	liq	BP	313.51	SEL		25.4	1.1	DvH eval	2019DIK
	2-pentyne	liq	BP	329.27	SEL		25.0	1.1	DvH eval	2019DIK
C_6H_{10}	1-hexyne	liq	BP	344.53	SEL		30.0	0.4	DvH eval	2019DIK
	2-hexyne	liq	BP	357.59	SEL	33.52	32.21		VP eval	2019DIK

	3-hexyne	liq	BP	354.58	SEL		31.6	0.4	DvH eval	2019DIK
Alkenynes										
C_4H_4	butenyne	gas	BP	279.18	SEL		23.9	0.7	DvH eval	2019DIK
C_5H_6	3-penten-1-yne	liq	BP	317.05	SEL		26.6	1.4	DvH eval	2019DIK
Alkadiynes										
C_4H_2	butadiyne	gas	BP	283.65	SEL		24.0	1.0	DvH eval	2019DIK
Cycloalkanes										
C_3H_6	cyclopropane	gas	BP	240.27	SEL		20.0	0.6	DvH eval	2019DIK
C_4H_8	cyclobutane	gas	BP	285.64	SEL		23.7	0.4	DvH eval	2019DIK
C_5H_{10}	cyclopentane	liq	BP	322.4	SEL		27.30	0.20	DvH	1959MCC2
	methylcyclobutane	liq	BP	310.0	SEL		25.3	1.2	DvH eval	2019DIK
C_6H_{12}	cyclohexane	liq	BP	353.8649	SEL		29.99	0.15		2014ZHO
	methylcyclopentane	liq	BP	344.96	SEL		29.07	0.10	DvH	1959MCC2
C_7H_{14}	1,1-dimethylcyclopentane	liq	BP	360.99	SEL	31.72	30.48		VP	1949FOR
	ethylcyclopentane	liq	BP	376.61	SEL	33.58	32.27		VP	1949FOR
	methylcyclohexane	liq	BP	374	SEL		31.23	na		2018LEM
C_8H_{16}	isopropylcyclopentane	liq	BP	399.57	SEL	35.56	34.17		VP	1949FOR
	n-propylcyclopentane	liq	BP	404.1	SEL	36.57	35.15		VP	1949FOR
C_9H_{18}	isopropylcyclohexane	liq	BP	427.71	SEL	38.41	36.91		VP	1949FOR
	propylcyclohexane	liq	BP	429.87	SEL	38.87	37.36		VP	1949FOR
$C_{10}H_{20}$	1,3-diethylcyclohexane	liq	BP	445.7	SEL		37.5	1.2	DvH eval	2019DIK
	isobutylcyclohexane	liq	BP	444.47	SEL	40.27	38.69		VP	1949FOR
	tert-butylcyclohexane	liq	BP	444.74	SEL	39.86	38.30		VP	1949FOR
Cycloalkenes										
C_3H_4	cyclopropene	gas	BP	237.7	SEL		20.50	0.60		2019DIK
C_4H_6	cyclobutene	gas	BP	275.73	SEL		23.19	0.46		2018LEM
C_5H_8	cyclopentene	liq	BP	317.39	SEL		26.9	0.4	DvH eval	2019DIK
	methylenecyclobutane	liq	BP	315.0	SEL		25.3	1.2	DvH eval	2019DIK
C_6H_{10}	cyclohexene	liq	BP	356.1	SEL		30.66	0.25	DvH	1973SVO
Cycloalkadienes										
C_5H_6	1,3-cyclopentadiene	liq	BP	314.7	SEL	25.00	24.02		VLE	1967LES
C_6H_8	1,3-cyclohexadiene	liq	BP	353.49	SEL	31.49	30.26		VP	1973MEY
Bicyclolalkanes										
$C_{10}H_{18}$	cis-decalin	liq	BP	468.93	SEL		39.9	0.4	DvH eval	2019DIK
	trans-decalin	liq	BP	460.42	SEL		38.9	0.4	DvH eval	2019DIK
$C_{12}H_{22}$	cyclohexylcyclohexane	liq	BP	511.1	SEL		43.86	0.28	DvH eval	2019DIK

	sol	MP	276.80	SEL1	6.86	MP	2002CHI

Table 3-3(3). Aromatic Hydrocarbons

Formula	Compound	Phase	trs	T_{trs} (K)	SEL	$\Delta_v H$(IG) ---	$\Delta_{trs}H$ (kJ mol^{-1})	unc ---	Method	Reference
Alkylbenzenes										
C_6H_6	benzene	liq	BP	353.22	SEL		30.75	0.06	EOS	2012THO
		sol	MP	278.67	SEL1		9.87	0.01	MP	1948OLI
C_7H_8	toluene	liq	BP	383.75	SEL		33.23	0.16	EOS	2006LEM
		sol	MP	178.15	SEL1		6.64	0.01	MP	1962SCO
C_8H_{10}	1,2-dimethylbenzene	liq	BP	417.521	SEL		36.38	0.18		2012CHO
	1,3-dimethylbenzene	liq	BP	412.214	SEL		36.11	0.07		2012CHO
	1,4-dimethylbenzene	liq	BP	411.47	SEL		35.71	0.07		2012CHO
	ethylbenzene	liq	BP	409.314	SEL		35.60	0.11		2012ZHO
C_9H_{12}	1,2,3-trimethylbenzene	liq	BP	449.23	SEL	41.95	40.31		VP	1949FOR
	1,2,4-trimethylbenzene	liq	BP	442.5	SEL	41.29	39.68		VP	1949FOR
	1,3,5-trimethylbenzene	liq	BP	437.87	SEL	41.12	39.52		VP	1949FOR
	2-ethyltoluene	liq	BP	438.25	SEL	40.70	39.11		VP	1949FOR
	3-ethyltoluene	liq	BP	434.46	SEL	40.40	38.83		VP	1949FOR
	4-ethyltoluene	liq	BP	435.14	SEL	40.24	38.67		VP	1949FOR
	isopropylbenzene	liq	BP	425.54	SEL		37.0	0.4	DvH eval	2019DIK
	n-propylbenzene	liq	BP	432.32	SEL	39.75	38.20		VP	1949FOR
$C_{10}H_{14}$	1,2-diethylbenzene	liq	BP	456.57	SEL	42.71	41.04		VP	1949FOR
	1,3-diethylbenzene	liq	BP	454.25	SEL	42.65	40.98		VP	1949FOR
	1,4-diethylbenzene	liq	BP	456.9	SEL	42.68	41.01		VP	1949FOR
	2-isopropyltoluene	liq	BP	451.5	SEL		39.3	0.7	DvH eval	2019DIK
	3-isopropyltoluene	liq	BP	448.35	SEL		39.3	0.7	DvH eval	2019DIK
	4-isopropyltoluene	liq	BP	450.27	SEL		39.3	0.4	DvH eval	2019DIK
	n-butylbenzene	liq	BP	456.42	SEL	42.53	40.87		VP	1949FOR
	tert-butylbenzene	liq	BP	442.27	SEL	40.61	39.03		VP	1949FOR
Alkenylbenzenes										
C_8H_8	ethenylbenzene	liq	BP	418.45	SEL		36.8	0.4	DvH eval	2019DIK
Benzocyclolkanes										
$C_{10}H_{12}$	benzocyclohexane	liq	BP	480.56	SEL		42.6	0.5	DvH eval	2019DIK
Benzocyclolkenes										

C_9H_8	benzocyclopentene	liq	BP	454.72	SEL		40.36	0.4	DvH eval	2019DIK
Alkylnapthalenes										
$C_{10}H_8$	naphthalene	sol	MP	353.40	SEL		18.993	0.019	MP	2002CHI
			BP	491.11	SEL1		43.3	0.8	DvH eval	2019DIK
			TP	353.37	SEL2		70.38	0.3	VP	2005RUZ
$C_{11}H_{10}$	1-methylnaphthalene	liq	BP	517.84	SEL		46.3	0.3	DvH eval	2019DIK
		sol	MP	242.65	SEL1		6.95		MP	1957MCC
	2-methylnaphthalene	sol	MP	307.70	SEL		12.13		MP rev	1996DOM
			BP	514.2	SEL1	48.23	46.35		VP	1955CAM
Polycyclic Aromatics										
$C_{12}H_8$	acenaphthylene	sol	MP	366.40	SEL		10.96		MP rev	1996DOM
		sol	MP	550.60	SEL1		46.4	2.4	DvH est	2019DIK
	biphenylene	sol	MP	384.40	SEL		82.7		DsubH est	1995NAS
			BP	548.50	SEL1		46.3	1.7	DvH est	2019DIK
$C_{12}H_{10}$	acenaphthene	sol	MP	364.02	SEL		21.46		MP	1977FIN
			BP	550.39	SEL1	53.88	51.78		VP	1923MOR
$C_{13}H_{10}$	fluorene	sol	MP	387.90	SEL		19.10		MP	2000LIS
			BP	570.19	SEL1	56.87	54.65		VP	1923MOR
$C_{14}H_{10}$	anthracene	sol	MP	489.50	SEL		29.37		MP	1970GOU
			BP	614.87	SEL1	58.54	56.25		VP	1923MOR
	phenanthrene	sol	MP	372.74	SEL		16.60		MP	2003ROJ
			BP	609.0	SEL1	59.56	57.24		VP	1975OSB
$C_{16}H_{10}$	fluoranthene	sol	MP	381.00	SEL		18.73		MP	1971WON
			BP	659.82	SEL1	51.46	49.45		VP	1955TSY
	pyrene	sol	MP	424.30	SEL		16.70		MP	2003ROJ
			BP	668.17	SEL1	56.54	54.34		VP	1955TSY
$C_{20}H_{12}$	perylene	sol	MP	550.90	SEL		32.58		MP	1992SAB
$C_{24}H_{12}$	coronene	sol	MP	710.50	SEL		21.20		MP	2009TOR

Table 3-3(4). Oxidized Hydrocarbons

Formula	Compound	Phase	trs	T_{trs} (K)	SEL	$\Delta_v H$(IG) ---	$\Delta_{trs} H$ (kJ mol^{-1})	unc ---	Method	Reference
Carbon Oxides										
CO_2	carbon dioxide	sol	SP	194.67	SEL		25.230	0.002	DsubH	1937GIA
		sol	TP	216.57	SEL1		25.64	0.25	TP eval	2019DIK
CO	carbon monoxide	gas	BP	81.64	SEL		6.01	0.02	EOS	2006LEM
Alkanols										
CH_4O	methanol	liq	BP	337.63	SEL		35.28	0.21	EOS	1993REU
C_2H_6O	ethanol	liq	BP	351.57	SEL		39.14	0.47	EOS	2014SCH
C_3H_8O	1-propanol	liq	BP	370.26	SEL		41.7	0.4	DvH eval	2019DIK
	isopropanol	liq	BP	354.4	SEL		40.04	0.25	DvH	1926MAT
$C_4H_{10}O$	1-butanol	liq	BP	390.77	SEL		42.9	0.5	DvH eval	2019DIK
	2-butanol	liq	BP	372.66	SEL	42.90	41.22		VP	1963BID
	isobutanol	liq	BP	381.04	SEL	44.01	42.29	0.40	VP	1963BID
	tert-butanol	sol	MP	298.87	SEL		6.78		MP	1926PAR
			BP	355.5	SEL1		39.15	0.22	DvH eval	2019DIK
			SP	298.15	SEL2		49	5	est	2022TWE
$C_5H_{12}O$	1-pentanol	liq	BP	410.9	SEL		44.2	0.6	DvH eval	2019DIK
	2-methyl-1-butanol	liq	BP	402.14	SEL		43.5	0.5	DvH eval	2019DIK
	2-pentanol	liq	BP	392.29	SEL	44.53	42.79		VP	1935BUT
	isopentanol	liq	BP	404.73	SEL		43.6	0.3	DvH eval	2019DIK
Glycols										
$C_2H_6O_2$	1,2-ethanediol	liq	BP	470.313	SEL		54.56	na		2018LEM
$C_3H_8O_2$	1,2-propanediol	liq	BP	461.22	SEL	53.58	51.49		VP	2002STE
	2-methoxyethanol	liq	BP	397.54	SEL		39.59	0.26	DvH eval	2019DIK
Sugars										
$C_3H_8O_3$	glycerin	liq	BP	563.0	SEL		63.3	1.5	DvH eval	2019DIK
		sol	MP	291.05	SEL1		18.29		MP	1923GIB
$C_6H_{12}O_6$	alpha-D-glucose	sol	MP	414	SEL		31.4		MP rev	2019DIK
		liq	BP	706	SEL1(u)		84.4	4.2	DvH est	2019DIK
		sol	SP	425	SEL2		194	5	VP	1990OJA

$C_{12}H_{22}O_{11}$	sucrose	sol	MP	424.4	SEL		32		cal	2014MAG
			SP	298.15	SEL2		94		est	2022TWE
			MP	456.40			46.20		MP	1988SOP
Phenols										
C_7H_8O	2-methylphenol	sol	MP	304.20	SEL		15.82		MP	1967AND
			BP	464.14	SEL1	46.53	44.71		VP	1949DRE
	4-methylphenol	sol	MP	307.84	SEL		12.71		MP	1967AND
			BP	474.99	SEL1	49.29	47.36		VP	1949DRE
Alkyl Ethers										
C_2H_6O	dimethyl ether	gas	BP	248.37	SEL		21.43	0.90	EOS	2011WU
$C_4H_{10}O$	diethyl ether	liq	BP	307.56	SEL		26.55	0.27	EOS	2014THO
$C_6H_{14}O$	diisopropyl ether	liq	BP	341.49	SEL		28.99	0.17	DvH eval	2019DIK
	di-n-propyl ether	liq	BP	363.25	SEL	33.16	31.86		VP	1973MEY
Aldehydes										
CH_2O	formaldehyde	gas	BP	254.13	SEL		22.0	0.4	DvH est	2019DIK
C_2H_4O	acetaldehyde	liq	BP	299.12	SEL		25.07	0.21	DvH eval	2019DIK
C_3H_6O	propanal	liq	BP	321.19	SEL		28.3	0.4	DvH eval	2019DIK
C_4H_8O	butanal	liq	BP	347.95	SEL(u)		29.32	0.28	DvH eval	2019DIK
	isobutanal	liq	BP	337.26	SEL	30.73	29.54		VP	1959SEP
Alkenals										
C_3H_4O	2-propenal	liq	BP	325.4	SEL		29.6	0.3	DvH eval	2019DIK
Ketones										
C_3H_6O	acetone	liq	BP	329.22	SEL		29.12	0.27	EOS	2006LEM
C_4H_8O	butanone	liq	BP	352.74	SEL		31.59	0.16	DvH eval	2019DIK
$C_5H_{10}O$	3-pentanone	liq	BP	375.11	SEL	35.31	33.93		VP	1965COL
Carboxylic Acids										
CH_2O_2	formic acid	liq	BP	374.05	SEL		22.7	8.4	DvH est	2019DIK
		sol	MP	281.47	SEL1		12.68		MP	1941STO
$C_2H_4O_2$	acetic acid	liq	BP	391.2	SEL	38.67	37.16		VLE	2019LI
		sol	MP	289.49	SEL1		11.72		MP	1982MAR
C_3H_6O	propanoic acid	liq	BP	413.99	SEL		29.91	0.7	DvH	1989JAS
C_4H_8O	n-butanoic acid	liq	BP	436.42	SEL		38.4	2.4	DvH eval	2019DIK
Alkyl Esters										
$C_2H_4O_2$	methyl formate	liq	BP	305.14	SEL		27.90	0.25	DvH	1976CIH
$C_3H_6O_2$	ethyl formate	liq	BP	327.29	SEL		29.80	0.20	DvH	1976CIH
$C_4H_8O_2$	ethyl acetate	liq	BP	349.2	SEL		32.30	0.30	DvH	1926MAT

Alkenyl Esters									
$C_4H_6O_2$	vinyl acetate	liq	BP	345.33	SEL		31.7	0.3	DvH eval	2019DIK
$C_5H_8O_2$	ethyl propenoate	liq	BP	372.59	SEL		34.2	0.4	DvH eval	2019DIK
	methyl 2-methylpropenoate	liq	BP	369.73	SEL		34.14	0.28	DvH eval	2019DIK
Oxacycloalkanes									
C_2H_4O	oxacyclopropane	gas	BP	283.59	SEL		25.47	0.19	EOS	2015THO
C_3H_6O	methyloxacyclopropane	liq	BP	307.268	SEL		27.59	0.14	EOS-rev	2018LEM
Oxacycloalkadienes									
C_4H_4O	oxacyclopentadiene	liq	BP	304.51	SEL		27.03	0.18	DvH eval	2019DIK
C_5H_6O	2-methyloxacyclopentadiene	liq	BP	338.39	SEL	30.86	29.66		VP	1971EON
Oxacycloketones									
C_4H_6O	cyclobutanone	liq	BP	367.79	SEL	37.15	35.70		VP	1942BEN
$C_6H_{10}O$	cyclohexanone	liq	BP	428.57	SEL	39.48	37.94		VP	1973MEY
Dioxanes and trioxanes									
$C_3H_6O_3$	1,3,5-trioxane	sol	MP	333.44	SEL		15.105	0.010	MP	1988VAN
			BP	387.2	SEL1		37.3	2.1	DvH est	2019DIK
			SP	298.15	SEL2		56.6	0.2	C	1969MAN
$C_3H_6O_3$	1,3,5-trioxane	sol	MP	333.65	SEL		15.105		MP	1988VAN
			BP	387.2	SEL1		37.3	2.1	DvH est	2019DIK
$C_4H_8O_2$	1,3-dioxane	liq	BP	378.13	SEL		34.3	2.4	DvH est	2019DIK
	1,4-dioxane	liq	BP	374.25	SEL		35.58	0.3	DvH	1963VIN
Furandione and D-Camphor									
$C_{10}H_{16}O$	D-camphor	sol	MP	463.38	SEL(u)		15.7		DfusH rev	1990DON
			BP	493.0	SEL1(u)		44.0	1.8	DvH est	2019DIK
			SP	298.15	SEL2		51.9	0.8	VP	1977STE
$C_4H_2O_3$	2,5-furandione	sol	MP	325.70	SEL		12.26		MP	1978MAR
			BP	478.33	SEL1		44.7	2.3	DvH est	2019DIK
			SP	319.0	SEL2		70.72	0.42	cal	2017SOU
Aromatic Alcohols									
C_6H_6O	phenol	sol	MP	314.05	SEL		11.54		MP	1963AND
			BP	454.91	SEL1		45.47	0.23	DvH eval	2019DIK
C_7H_8O	3-methylphenol	liq	BP	475.28	SEL		47.2	0.5	DvH eval	2019DIK
		sol	MP	285.37	SEL1		10.67		MP	1998JAM
	benzyl alcohol	liq	BP	477.4	SEL		50.49	1.00	DvH	1926MAT
Aromatic Aldehydes and Acids									
C_7H_6O	Benzaldehyde	liq	BP	451.15	SEL		40.9	0.3	DvH eval	2019DIK

$C_7H_6O_2$	benzoic acid	sol	MP	395.50	SEL	17.10		MP	2002ROY
			BP	523.53	SEL1	56.5	1.0	DvH eval	2019DIK
			SP	298.15	SEL2	89.25	0.42	VP	1990DAS

Table 3-3(5). Nitrogen-Substituted Hydrocarbons

Formula	Compound	Phase	trs	T_{trs} (K)	SEL	$\Delta_v H$(IG) ---	$\Delta_{trs} H$ (kJ mol^{-1})	unc ---	Method	Reference
Hydrogen Cyanides										
CHN	hydrogen cyanide	liq	BP	298.79	SEL		25.22	0.25	DvH eval	2019DIK
Alkyl Amines										
CH_5N	methylamine	gas	BP	266.84	SEL		25.94	0.23	DvH eval	2019DIK
C_3H_9N	n-propylamine	liq	BP	320.38	SEL		29.58	0.20	DvH eval	2019DIK
	isopropylamine	liq	BP	304.92	SEL	29.03	27.90		VP	1968OSB
$C_4H_{11}N$	n-butylamine	liq	BP	350.12	SEL		32.03	0.27	DvH eval	2019DIK
	tert-butylamine	liq	BP	317.19	SEL	29.53	28.38		VP	1968OSB
C_2H_7N	dimethylamine	gas	BP	280.02	SEL		26.48	0.06	DvH	1939AST
C_3H_9N	methylethylamine	liq	BP	305.6	SEL		28.4	0.5	DvH eval	2019DIK
	trimethylamine	gas	BP	276.0	SEL		23.00	0.22	DvH eval	2019DIK
$C_6H_{15}N$	triethylamine	liq	BP	361.93	SEL		31.3	0.4	DvH eval	2019DIK
Cycloalkylamines										
$C_6H_{13}N$	cyclohexylamine	liq	BP	406.98	SEL		35.8	0.6	DvH eval	2019DIK
Azacycloalkanes										
C_4H_9N	azacyclopentane	liq	BP	359.71	SEL	34.33	32.99		VP	1959MCC
$C_5H_{11}N$	azacyclohexane	liq	BP	379.37	SEL	35.14	33.77		VP	1968OSB
Methenamines										
$C_6H_{12}N_4$	methenamine	sol	SP	298.15	SEL		79.64	0.18	VP	2002VER
Azacycloalkadienes										
C_4H_5N	azacyclopentadiene	liq	BP	402.93	SEL	40.33	38.76		VP	1968OSB
C_5H_7N	1-methylazacyclopentadiene	liq	BP	385.9	SEL	36.82	35.38		VP	1968OSB
Alkanenitriles										
C_2H_3N	ethanenitrile	liq	BP	355.05	SEL		30.7	0.3	DvH eval	2019DIK
C_3H_5N	propanenitrile	liq	BP	370.73	SEL		33.0	0.4	DvH eval	2019DIK
C_4H_7N	butanenitrile	liq	BP	390.77	SEL		34.70	0.24	DvH eval	2019DIK
C_5H_9N	pentanenitrile	liq	BP	414.42	SEL	38.54	37.04		VP	1949DRE
$C_6H_{11}N$	hexanenitrile	liq	BP	436.61	SEL	41.24	39.63		VP	1973MEY
C_3H_3N	propenenitrile	liq	BP	351.13	SEL(u)		30.7	0.7	DvH eval	2019DIK
C_2N_2	cyanogen	gas	BP	252.0	SEL(u)		24.7	0.6	DvH eval	2019DIK

$C_2H_8N_2$	1,1-dimethylhydrazine	liq	BP	335.57	SEL		32.1	0.9	DvH eval	2019DIK
Melamines										
$C_3H_6N_6$	melamine	liq	SP	497	SEL		120	4	VP	1960HIR
			BP	639	SEL1		79	4	DvH est	2019DIK
Anilines										
C_6H_7N	2-methylpyridine	liq	BP	402.52	SEL	37.75	36.28		VP	1963SCO
	aniline	liq	BP	457.3	SEL		43.8	0.5	DvH eval	2019DIK
$C_8H_{11}N$	N,N-dimethylaniline	liq	BP	466.47	SEL		42.7	0.8	DvH eval	2019DIK
		sol	MP	275.65	SEL1		11.56		MP	1972AHM
Oxidized Amines										
CH_4N_2O	urea	sol	MP	406.5	SEL		14.79		MP	1987DEL
			SP	298.15	SEL1		94.6	2.0	VP	2003ZAI
$C_6H_{15}NO_3$	triethanolamine	liq	BP	623.15	SEL		82.0	2.0	VP	2004WRI
Alkyl Nitrates and Nitroalkanes										
CH_3NO_3	methyl nitrate	liq	BP	338.0	SEL(u)		26.4	1.4	DvH est	2019DIK
$C_3H_5N_3O_9$	nitroglycerin	sol	MP	286.65	SEL		21.87		MP rev	1991ACR
CN_4O_8	tetranitromethane	liq	BP	397.95	SEL		40.74		DvH rev	1985MAJ
		sol	SP	287.05	SEL1	47.40			DsubH	1941SEK
CH_3NO_2	nitromethane	liq	BP	373.1	SEL		34.46	0.30	DvH	1926MAT
Isocyanates										
$C_9H_6N_2O_2$	2,4-diisocyanatotoluene	liq	BP	524.83	SEL(u)		41.9	2.1	DvH est	2019DIK
Nitro Aromatics										
$C_6H_5NO_2$	nitrobenzene	liq	BP	483.81	SEL		43.9	0.5	DvH eval	2019DIK
		sol	MP	278.89	SEL1		12.12		MP	1936PAR
$C_7H_5N_3O_6$	trinitrotoluene	sol	MP	355.1	SEL		23.43		DfusH	1993ACR
			BP	620.5	SEL1	73.69			VP	1948ROB
			SP	298.15	SEL2		113.2	1.5	VP	1979KUD

Table 3-3(6). Sulfur-Substituted Hydrocarbons

Formula	Compound	Phase	trs	T_{trs} (K)	SEL	$\Delta_v H$(IG) ---	$\Delta_{trs} H$ (kJ mol^{-1})	unc ---	Method	Reference
Alkanethiols										
CH_4S	methanethiol	gas	BP	279.05	SEL		24.4	0.9	DvH eval	2019DIK
C_2H_6S	ethanethiol	liq	BP	308.19	SEL		26.6	0.6	DvH eval	2019DIK
C_3H_8S	1-propanethiol	liq	BP	340.87	SEL	30.80	29.60		VP	1956PEN
	isopropanethiol	liq	BP	325.71	SEL	29.12	27.99		VP	1966OSB
$C_4H_{10}S$	1-butanethiol	liq	BP	371.56	SEL	33.79	32.47		VP	1966OSB
	1-isobutanethiol	liq	BP	361.64	SEL	32.48	31.22		VP	1966OSB
	2-butanethiol	liq	BP	358.13	SEL	32.04	30.79		VP	1966OSB
$C_5H_{12}S$	1,1-dimethyl-1-propanethiol	liq	BP	372.28	SEL	32.95	31.66		VP	1966OSB
	1-pentanethiol	liq	BP	399.79	SEL	36.69	35.26		VP	1966OSB
$C_6H_{14}S$	1-hexanethiol	liq	BP	425.81	SEL	39.46	37.92		VP	1966OSB
$C_7H_{16}S$	1-heptanethiol	liq	BP	450.07	SEL	42.15	40.50		VP	1966OSB
Alkyl Sulfides										
CS_2	carbon disulfide	liq	BP	318.4	SEL		26.78	0.15	DvH	1926MAT
$C_2H_6S_2$	dimethyl disulfide	liq	BP	382.89	SEL	34.98	33.61		VP	1950SCO
C_2H_6S	dimethyl sulfide	liq	BP	310.42	SEL		27.0	0.3	DvH eval	2019DIK
C_3H_8S	ethyl methyl sulfide	liq	BP	339.8	SEL	30.78	29.58		VP	1952WHI
$C_4H_{10}S$	diethyl sulfide	liq	BP	365.25	SEL	33.26	31.97		VP	1966OSB
Thiacycloalkanes										
C_4H_8S	thiacyclopentane	liq	BP	394.27	SEL	35.94	34.53		VP	1966OSB
Thiacycloalkenes										
C_4H_4S	thiacyclopentadiene	liq	BP	357.31	SEL	32.63	31.35		VP	1949WAD
Aromatic Thiols										
C_6H_6S	benzenethiol	liq	BP	442.29	SEL	41.35	39.74		VP	1966OSB
Alkyl Sulfoxides										
C_2H_6OS	dimethyl sulfoxide	liq	BP	463.86	SEL		43.5	0.4	DvH eval	2019DIK
		sol	MP	291.57	SEL1		14.37		MP	1970CLE

Table 3-3(7). Halogenated Hydrocarbons

Formula	Compound	Phase	trs	T_{trs} (K)	SEL	$\Delta_v H$(IG) ---	$\Delta_{trs}H$ (kJ mol^{-1})	unc ---	Method	Reference
Fluoroalkanes										
CH_3F	fluoromethane	gas	BP	194.65	SEL		16.60	0.46	EOS	2006LEM
CH_2F_2	difluoromethane	gas	BP	221.5	SEL		19.87	0.20	EOS	1997TIL
CHF_3	trifluoromethane	gas	BP	188.75	SEL		16.76	0.15	EOS	2003PEN
CF_4	tetrafluoromethane	gas	BP	145.56	SEL		11.83	0.27	EOS	1990PLA
C_2H_5F	fluoroethane	gas	BP	236.05	SEL		20.26	0.04	EOS	2016QI
$C_2H_4F_2$	1,1-difluoroethane	gas	BP	249.13	SEL		21.79	0.72	EOS	1996OUT
$C_2H_3F_3$	1,1,1-trifluoroethane	gas	BP	225.91	SEL		19.05	0.56	EOS	2000LEM
	1,1,2-trifluoroethane	gas	BP	276.81	SEL(u)		25.7	0.4	DvH est	2019DIK
$C_2H_2F_4$	1,1,1,2-tetrafluoroethane	gas	BP	247.08	SEL		22.138	0.004	EOS	1994LIL
	1,1,2,2-tetrafluoroethane	gas	BP	253.23	SEL		22.7	1.0	DvH eval	2019DIK
C_2HF_5	pentafluoroethane	gas	BP	225.06	SEL		19.70	0.22	EOS	2005LEM
C_2F_6	hexafluoroethane	gas	BP	194.87	SEL		16.14	0.05	EOS	2006LEM
Fluoroalkenes										
C_2H_3F	fluoroethene	gas	BP	201.65	SEL(u)		16.2	1.0	DvH est	2019DIK
$C_2H_2F_2$	1,1-difluoroethene	gas	BP	190.15	SEL		14.9	0.4	DvH eval	2019DIK
	1,2-difluoroethene, €-	gas	BP	231.15	SEL(u)		20.6	1.1	DvH est	2019DIK
	1,2-difluoroethene, (Z)-	gas	BP	253.15	SEL(u)		16.4	0.9	DvH est	2019DIK
C_2HF_3	trifluoroethene	gas	BP	211.7	SEL(u)		20.35	0.90	EOS	2016AKA
C_2F_4	tetrafluoroethene	gas	BP	197.51	SEL		16.83	0.15	DvH eval	2019DIK
Chloroalkanes										
CH_3Cl	chloromethane	gas	BP	249.0	SEL		21.61	0.41	EOS	2014THO
CH_2Cl_2	dichloromethane	liq	BP	312.92	SEL		27.95	0.20	DvH	1976DEP
$CHCl_3$	trichloromethane	liq	BP	333.3	SEL		29.37	0.25	DvH	1926MAT
CCl_4	tetrachloromethane	liq	BP	348.6	SEL		29.96	0.40	DvH	1926MAT
C_2H_5Cl	chloroethane	gas	BP	285.4	SEL		24.42	0.14	DvH eval	2019DIK
$C_2H_4Cl_2$	1,1-dichloroethane	liq	BP	330.42	SEL		29.02	0.16	DvH eval	2019DIK
	1,2-dichloroethane	liq	BP	356.7	SEL		32.090	0.032	EOS	2017THO
$C_2H_3Cl_3$	1,1,1-trichloroethane	liq	BP	347.22	SEL(u)		29.69	0.20	DvH eval	2019DIK
	1,1,2-trichloroethane	liq	BP	386.78	SEL		34.94	0.23	DvH eval	2019DIK

$C_2H_2Cl_4$	1,1,1,2-tetrachloroethane	liq	BP	403.33	SEL		35.07	0.27	DvH eval	2019DIK
	1,1,2,2-tetrachloroethane	liq	BP	419.25	SEL(u)		38.0	0.8	DvH eval	2019DIK
C_2HCl_5	pentachloroethane	liq	BP	433.45	SEL(u)		37.4	1.8	DvH est	2019DIK
C_2Cl_6	hexachloroethane	sol	MP	458.15	SEL		9.75		MP rev	1996DOM
			BP	458.2	SEL1(u)		37.5	1.5	DvH est	2019DIK
			SP	439	SEL2		59.0	0.8	VP	1947IVI
Chloroalkenes										
C_2H_3Cl	chloroethene	gas	BP	259.443	SEL		22.31	0.07		2018LEM
$C_2H_2Cl_2$	1,1-dichloroethene	liq	BP	304.71	SEL		26.46	0.26	DvH eval	2019DIK
	1,2-dichloroethene, €-	liq	BP	320.73	SEL		27.9	0.4	DvH eval	2019DIK
	1,2-dichloroethene, (Z)-	liq	BP	333.58	SEL		29.62	0.29	DvH eval	2019DIK
C_2HCl_3	trichloroethene	liq	BP	358.8	SEL		31.47	0.25	DvH	1926MAT
C_2Cl_4	tetrachloroethene	liq	BP	394.29	SEL		34.41	0.24	DvH eval	2019DIK
Chloroaromatics										
C_6H_5Cl	chlorobenzene	liq	BP	405.21	SEL		35.53	0.44	EOS-rev	2018LEM
Bromoalkanes										
CH_3Br	bromomethane	gas	BP	276.7	SEL		23.5	0.5	DvH eval	2019DIK
CH_2Br_2	dibromomethane	liq	BP	370.1	SEL		33.4	0.4	DvH eval	2019DIK
$CHBr_3$	tribromomethane	liq	BP	422.36	SEL		37.5	0.3	DvH eval	2019DIK
CBr_4	tetrabromomethane	sol	MP	367.60	SEL		3.95		MP rev	1996DOM
			BP	462.55	SEL1	40.95	39.35		VP	1947STU
			SP	298.15	SEL2		54.5	0.7	cal	1984BIC
C_2H_5Br	bromoethane	liq	BP	311.54	SEL		26.9	0.3	DvH eval	2019DIK
Bromoalkenes										
C_2H_3Br	bromoethene	liq	BP	311.54	SEL(u)		27.3	1.9	DvH est	2019DIK
Chlorofluoromethanes										
CH_2ClF	chlorofluoromethane	gas	BP	264.0	SEL(u)		19.7	1.1	DvH est	2019DIK
$CHClF_2$	chlorodifluoromethane	gas	BP	232.35	SEL		20.21	0.19	EOS	1995KAM
$CHCl_2F$	dichlorofluoromethane	gas	BP	282.05	SEL		24.64	0.20	EOS	1990PLA
$CClF_3$	chlorotrifluoromethane	gas	BP	191.75	SEL		15.601	0.016	EOS	2000MAG
CCl_2F_2	dichlorodifluoromethane	gas	BP	243.35	SEL		20.09	0.04	EOS	1992MAR
CCl_3F	trichlorofluoromethane	gas	BP	296.858	SEL		24.91	0.05	EOS	2000JAC
C_2ClF_3	chlorotrifluoroethene	gas	BP	244.8	SEL		20.71	0.25	DvH eval	2019DIK
Bromofluoroalkanes										
CH_2BrF	bromofluoromethane	liq	BP	310.0	SEL(u)		30.6	1.6	DvH est	2019DIK
$CHBrF_2$	bromodifluoromethane	gas	BP	258.65	SEL		22.5	1.0	DvH eval	2019DIK

$CBrF_3$	bromotrifluoromethane	gas	BP	215.35	SEL		17.48	0.17	DvH eval	2019DIK
CBr_2F_2	dibromodifluoromethane	gas	BP	297.65	SEL		24.45	0.19	DvH eval	2019DIK
CBr_3F	tribromofluoromethane	liq	BP	379.65	SEL(u)		42.6	2.1	DvH est	2019DIK
Bromochloroalkanes										
CH_2BrCl	bromochloromethane	liq	BP	341.21	SEL		30.55	0.18	DvH eval	2019DIK
$CHBrCl_2$	bromodichloromethane	liq	BP	362.65	SEL(u)		31.8	1.7	DvH est	2019DIK
$CHBr_2Cl$	dibromochloromethane	liq	BP	393.0	SEL(u)		38.4	1.9	DvH est	2019DIK
$CBrCl_3$	bromotrichloromethane	liq	BP	376.65	SEL(u)		32.1	1.4	DvH est	2019DIK
CBr_2Cl_2	dibromodichloromethane	liq	BP	423.35	SEL(u)		34.1	1.8	DvH est	2019DIK
Bromochlorofluoroalkanes										
CHBrClF	bromochlorofluoromethane	liq	BP	312.6	SEL(u)		26.9	1.4	DvH est	2019DIK
$CBrClF_2$	bromochlorodifluoromethane	gas	BP	270.65	SEL		22.15	0.10	DvH eval	2019DIK
$CBrCl_2F$	bromodichlorofluoromethane	liq	BP	325.15	SEL(u)		29.5	1.6	DvH est	2019DIK
CBr_2ClF	dibromochlorofluoromethane	liq	BP	352.65	SEL(u)		32.9	1.7	DvH est	2019DIK
Carbonyl Halides										
CF_2O	carbonyl difluoride	gas	BP	188.58	SEL	18.92			VP	1968PAC
CCl_2O	phosgene	gas	BP	280.71	SEL		24.40	0.05	DvH	1948GIA
Chlorophenols										
C_6HCl_5O	pentachlorophenol	sol	MP	462.80	SEL		17.15		MP rev	1991ACR
			BP	582.5	SEL1(u)		59.1	2.8	DvH est	2019DIK
			SP	298.15	SEL2		91.64	0.22	VP	2007VER

Table 3-3(8). Siloxanes

Formula	Compound	Phase	trs	T_{trs} (K)	SEL	$\Delta_v H$(IG) ---	$\Delta_{trs} H$ (kJ mol^{-1})	unc ---	Method	Reference
$C_6H_{18}Osi_2$	hexamethyldisiloxane	liq	BP	373.66	SEL(u)		31.32		DvH	2011ABB
$C_8H_{24}O_4Si_4$	octamethylcyclotetrasiloxane	liq	BP	448.02	SEL(u)		38.4	1.2	DvH eval	2019DIK
		sol	MP	290.65	SEL1		23.77		MP rev	1996DOM

3.3.2. **Discussion of Uncertainties in Heats of Vaporization**

As discussed earlier, in Section 3.1, we derived an average compressibility factor of 0.961 ± 0.0055 (1σ), or an uncertainty of only about 0.6 %; this is less than the uncertainties in experimental determinations of latent enthalpies of vaporization, which are on the order of (1 to 2) %. We used this compressibility factor to estimated corrected real gas enthalpies of vaporization $\Delta_v H$ from ideal gas enthalpies of vaporization $\Delta_v H$(IG), derived using vapor pressure curves ln(P) vs. (1/T).

A good source of normal boiling points and latent enthalpies of vaporizations for reference fluids can be found in REFPROP[2018LEM]. It does not, however, explicitly provide uncertainties in normal boiling points or enthalpies of vaporization, but can be derived from other information contained in REFPROP. Table 3-3(9) below provides normal boiling points and enthalpies of vaporization along with uncertainties for 75 compounds in NIST REFPROP (plus formic acid and 1,2-propanediol from NIST TRC TDE).[2019DIK] The change in pressure with temperature $\delta P/\delta T$ at the normal boiling point is also given. The uncertainties in normal boiling points were calculated using the uncertainties in pressure and $\delta P/\delta T$ as provided in NIST REFPROP (or TDE). Note here that we use the infinitesimal change notations $\delta P/\delta T$, $\delta\ln(P/P_0$, and $\delta(1/T)$ since the values were computed numerically rather than the analytical derivative notations dP/dT, dln(P/P0), and d(1/T).

Considering the equation for enthalpies (heats) of vaporization:

(3.5) $\Delta_v H = -R\ \delta\ln(P/P_0)/\delta(1/T)$

(3.6) $U(\Delta_v H) \approx c\ R\ U(T)$

where c is a proportionality constant, and R is the gas constant.

We considered all of the 77 compounds in Table 3-3(9) and calculated the uncertainties in the enthalpies of vaporization $U(\Delta_v H)$ using:

(3.7) $\Delta_v H = -R\ \delta\ln(P/P_0)/\delta(1/T)$

(3.8) $\Delta_v H = -R\ \Delta\ln(P)\ /\ \Delta(1/T)$

(3.9) $\Delta_v H = -R\ \{\ln(P_1)-\ln(P_0)\}\ /\ (1/T_1 - 1/T_o)$

where T_1 *and* T_o were derived from the boiling points T_b for each compound using $\pm U(P) = \pm\Delta P =$ and $U(\Delta_v H)$ was then determined from the difference.

(3.10) $U(\Delta_v H) = -R\ [\ln(\Delta P) - \ln(-\Delta P)]\ /\ \Delta(1/T) - \Delta_v H$

In our analysis, we excluded a number of compounds that had large relative deviations, see Table 3-3(9) which identifies the outliers. Each of these compounds is a special case. Hydrogen has very low boiling temperature, formic acid forms dimers in the gas phase,

and thus, it is an extremely non-ideal gas with a compressibility factor Z of about 0.6 at the normal boiling point.[1999MIY] For *n*-undecane, *n*-dodecane and *n*-hexadecane, the uncertainties in the normal boiling temperatures are likely much higher than those computed from the estimated uncertainty in pressure (provided in NIST REFPROP)[2018LEM] of (0.2 %) and $U(P)/(\delta P/\delta T)$ – or $U(T_b)$ of (0.5 to 1.5) K versus 0.1 K; correspondingly, the uncertainties in enthalpies of vaporization would also be much higher than computed in the same fashion – or $U(\Delta_v H)$ of (1 to 2) kJ mol^{-1} versus 0.2 kJ mol^{-1}: a factor of (5 to 10) higher.

Overall, the relative expanded uncertainties in the enthalpies of vaporization are about $U(\Delta_v H)/\Delta_v H$ = (4.5±2.0) %

We now derive an entropic component. Trouton's Rule says that the molar entropy of vaporization for all liquids at their boiling points is approximately the same and can be used to estimate enthalpies of vaporization from normal boiling points: $S_b = \Delta_v H/T_b \approx$ (85 to 88) J mol^{-1} K^{-1}.[1884TRO] The entropy of vaporization ΔS_b is the difference between the entropy in the gas phase and that in the liquid phase $S_b = S_{gas} - S_{liq}$. However, $S_{gas} >> S_{liq}$, and, consequently, the entropy of vaporization is a measure of the cohesive energy holding the molecules together in the liquid phase. For small molecules, such as for hydrogen, methane, oxygen, and nitrogen, this energy is less and the entropy of vaporization is less – about (44.4, 73.4, and 75.6, and 82.1) J mol^{-1} K^{-1}, respectively, see Table 3-3(9). Increased order in the liquid phase and increased order in the gas phase increase and decrease the entropy of vaporization, respectively. For polar molecules, where there is hydrogen bonding (ordered structure) in the liquid phase, such as for ethanol, water, and ammonia, this energy is more and the entropy of vaporization is more – about (111.3, 108.9, and 97.3) J mol^{-1} K^{-1}, respectively. In contrast, for some molecules, there is hydrogen bonding (ordered structure) in the gas phase, such as for dimers; thus, the entropy of vaporization is less – for example, about 60.6 J mol^{-1} K^{-1} for formic acid. Water is a special case, where there is both hydrogen bonding in the liquid and gas phases – consequently, the entropy of vaporization of water of 108.9 J mol^{-1} K^{-1} is less than that for ethanol, because of the offset due to hydrogen bonding of water in the gas phase.

From our analysis, we find a simple relationship that predicts uncertainties to within about U = 4 %:

(3.11) $U(\Delta_v H)$ [kJ mol^{-1}] = $(\Delta_v H/T_b)^2/S_{b0}^2 / (\delta P/\delta T)$, or

(3.12) $U(\Delta_v H)$ [kJ mol^{-1}] = $(S_b^2/S_{b0}^2) / (\delta P/\delta T)$

where, $\Delta_v H$ is the heat of vaporization, T_b is the normal boiling point, $(\delta P/\delta T)$ is the change in pressure P with temperature, $S_b = \Delta_v H/T_b$ is the latent entropy of vaporization, and S_{b0} = 87.22 J mol^{-1} K^{-1} is the reference entropy of vaporization at the boiling point as determined from a least-squares fit to this expression. Here, S_{b0} is statistically identical to Trouton's Rule from 140 years ago).

Table 3-3(9). Derived uncertainties in EOS boiling points

This table provides boiling points (T_b), change in pressure with temperature ($\delta P/\delta T$), latent enthalpy of vaporization ($\Delta_v H$), Trouton's Rule entropy of vaporization ($S_b = \Delta_v H/T_b$), along with expanded uncertainties U for boiling points, pressures, and heats of vaporization. The quantities T_b, $U(P)$, $\delta P/\delta T$, and $\Delta_v H$ were taken from NIST REFPROP.[2018LEM] $U(T_b)$ was calculated from $U(P)$ and $\delta P/\delta T$. $U(\Delta_v H)$ was computed (see text). $U(P)$ values that are underlined were not taken from NIST REFPROP estimates but taken directly from uncertainties provided in the literature. $U(P)$ for 1,2-dimethylbenzene was assigned the same as for the other two dimethylbenzenes. Note: a legend for the column headings is given in Table 3-3(11). Those compounds whose Trouton's rule S_b entropies of vaporization differ substantially are provided in **bold** in this table. The low S_b values are for the small, largely non-polar molecules reflects that lack of cohesive energy in the liquid state, while the high values are for largely polar molecules, where there is hydrogen bonding in the liquid phase. Those compounds whose uncertainties in enthalpy of vaporization are relatively high are provided in ***bold italics*** in this table.

Compound	T_b (K)	$U(T_b)$ (K)	$U(P)$ (atm)	$\delta P/\delta T$ (atm K^{-1})	$\Delta_v H$ (kJ mol^{-1})	$U(\Delta_v H)$ (kJ mol^{-1})	$U/\Delta_v H$ %	S_b (J mol^{-1} K^{-1})
hydrogen	20.369	0.007	0.002	0.295	0.91	0.11	***12.4%***	**44.4**
nitrogen	77.355	0.002	0.0002	0.118	5.58	0.29	5.2%	**72.1**
carbon monoxide	81.640	0.002	0.0002	0.114	6.01	0.31	5.1%	**73.7**
oxygen	90.1878	0.0143	0.0015	0.105	6.82	0.28	4.1%	**75.6**
methane	111.667	0.004	0.0003	0.082	8.20	0.30	3.7%	**73.4**
tetrafluoromethane	145.10	0.07	0.005	0.070	11.83	0.42	3.6%	81.5
ethene	169.379	0.008	0.0005	0.059	13.53	0.54	4.0%	79.9
ethane	184.566	0.002	0.0001	0.054	14.72	0.57	3.9%	79.7
nitrous oxide	184.68	0.03	0.002	0.060	16.47	0.54	3.3%	89.2
hydrogen chloride	188.173	0.088	0.005	0.057	16.18	0.60	3.7%	86.0
trifluoromethane	191.13	0.03	0.002	0.058	16.76	0.86	5.1%	87.7
chlorotrifluoromethane	191.67	0.02	0.001	0.054	15.60	0.89	5.7%	81.4
fluoromethane	194.84	0.05	0.0025	0.055	16.60	0.76	4.6%	85.2
hexafluoroethane	195.06	0.06	0.003	0.054	16.14	0.94	5.8%	82.7
hydrogen sulfide	212.85	0.05	0.0025	0.051	18.62	0.59	3.2%	87.5
trifluoroethene	214.06	0.02	0.001	0.056	20.35	0.98	4.8%	95.0
difluoromethane	221.499	0.004	0.0002	0.051	19.87	0.93	4.7%	89.7
pentafluoroethane	225.06	0.02	0.001	0.049	19.70	0.93	4.7%	87.5
propene	225.531	0.004	0.0002	0.045	18.47	0.56	3.0%	81.9
1,1,1-trifluoroethane	225.91	0.02	0.001	0.047	19.05	0.89	4.7%	84.3
propane	231.039	0.045	0.002	0.044	18.77	0.76	4.0%	81.2
chlorodifluoromethane	232.35	0.04	0.002	0.047	20.21	0.89	4.4%	87.0

fluoroethane	235.61	0.04	0.002	0.046	20.26	0.97	4.8%	86.0
ammonia	239.832	0.010	0.0005	0.050	23.33	0.58	2.5%	**97.3**
allene	240.87	0.12	0.0053	0.043	19.98	0.76	3.8%	82.9
dichlorodifluoromethane	243.40	0.05	0.002	0.043	20.09	1.09	5.4%	82.5
1,1,1,2-tetrafluoroethane	247.076	0.004	0.0002	0.046	22.14	1.21	5.5%	89.6
dimethyl ether	248.37	0.05	0.002	0.044	21.43	1.14	5.3%	86.3
1,1-difluoroethane	249.13	0.00	0.0002	0.046	22.14	1.60	7.2%	88.9
chloromethane	249.17	0.05	0.002	0.044	21.61	1.10	5.1%	86.7
propyne	250.00	0.09	0.004	0.045	22.60	0.78	3.5%	90.4
chloroethene	259.44	0.07	0.003	0.041	22.31	0.63	2.8%	86.0
isobutane	261.40	0.05	0.002	0.039	21.22	0.94	4.4%	81.2
sulfur dioxide	263.137	0.044	0.002	0.045	24.96	0.95	3.8%	94.8
isobutene	266.15	0.08	0.003	0.039	21.97	1.00	4.5%	82.6
1-butene	266.84	0.06	0.0025	0.039	22.01	1.08	4.9%	82.5
n-butane	272.66	0.01	0.0002	0.038	22.42	1.07	4.8%	82.2
2-butene, (*E*)-	274.03	0.08	0.003	0.038	22.73	0.99	4.4%	83.0
cyclobutene	275.73	0.18	0.007	0.038	23.19	0.83	3.6%	84.1
2-butene, (*Z*)-	276.87	0.05	0.002	0.038	23.24	0.98	4.2%	83.9
1-butyne	281.23	0.05	0.002	0.039	24.70	0.94	3.8%	87.8
dichlorofluoromethane	282.01	0.13	0.005	0.039	24.64	1.15	4.7%	87.4
neopentane	282.65	0.03	0.001	0.036	22.78	1.13	5.0%	80.6
oxacyclopropane	283.66	0.05	0.002	0.039	25.47	0.62	2.4%	89.8
trichlorofluoromethane	296.858	0.057	0.002	0.035	24.91	0.73	2.9%	83.9
isopentane	300.98	0.02	0.0007	0.035	24.77	1.59	6.4%	82.3
1-pentene	303.101	0.011	0.0004	0.035	25.21	1.52	6.0%	83.2
methyloxacyclopropane	307.268	0.028	0.001	0.036	27.59	0.67	2.4%	89.8
diethyl ether	307.56	0.11	0.004	0.036	26.55	1.76	6.6%	86.3
n-pentane	309.21	0.06	0.002	0.034	25.81	1.22	4.7%	83.5
cyclopentane	322.40	0.03	0.001	0.033	27.30	1.22	4.5%	84.7
neohexane	322.85	0.06	0.002	0.032	26.41	1.32	5.0%	81.8
acetone	329.22	0.07	0.0025	0.034	29.12	1.52	5.2%	88.5
2,3-dimethylbutane	331.18	0.06	0.002	0.032	27.55	1.63	5.9%	83.2
isohexane	333.36	0.06	0.002	0.032	27.84	1.73	6.2%	83.5
methanol	337.63	0.01	0.0005	0.039	35.28	1.68	4.8%	**104.5**
n-hexane	341.87	0.06	0.002	0.031	28.88	1.24	4.3%	84.5
ethanol	351.57	0.01	0.0005	0.039	39.14	0.94	2.4%	**111.3**

benzene	353.219	0.006	0.0002	0.031	30.75	1.41	4.6%	87.1
cyclohexane	353.87	0.02	0.0005	0.030	29.99	1.24	4.1%	84.8
1,2-dichloroethane	356.65	0.03	0.001	0.031	32.09	0.69	2.2%	90.0
n-heptane	371.55	0.07	0.002	0.029	31.73	1.55	4.9%	85.4
water	373.124	0.007	0.00025	0.036	40.65	1.02	2.5%	**108.9**
methylcyclohexane	374.00	0.09	0.0026	0.028	31.23	1.33	4.3%	83.5
formic acid	374.345	0.292	0.007	0.024	22.70	5.26	***23.2%***	**60.6**
toluene	383.75	0.02	0.0005	0.028	33.23	1.05	3.2%	86.6
n-octane	398.794	0.071	0.002	0.028	34.44	2.58	7.5%	86.4
chlorobenzene	405.21	0.11	0.003	0.027	35.53	1.33	3.7%	87.7
ethylbenzene	409.31	0.11	0.003	0.027	35.60	2.01	5.6%	87.0
1,4-dimethylbenzene	411.47	0.07	0.002	0.027	35.71	2.30	6.4%	86.8
1,3-dimethylbenzene	412.214	0.074	0.002	0.027	36.11	2.03	5.6%	87.6
1,2-dimethylbenzene	417.52	0.08	*0.002*	0.026	36.38	1.30	3.6%	87.1
n-nonane	423.91	0.08	0.002	0.026	37.01	1.83	5.0%	87.3
n-decane	447.27	0.08	0.002	0.025	39.33	2.25	5.7%	87.9
1,2-propanediol	461.224	0.033	0.001	0.030	47.91	5.15	***10.7%***	**103.9**
***n*-undecane**	468.93	0.08	0.002	0.025	41.43	4.28	***10.3%***	88.3
1,2-ethanediol	470.313	0.033	0.001	0.030	54.56	0.61	1.1%	**116.0**
***n*-dodecane**	489.44	0.08	0.002	0.024	43.63	4.17	***9.6%***	89.1
***n*-hexadecane**	559.90	0.09	0.002	0.022	51.75	5.59	***10.8%***	92.4

Table 3-3(10). Legend for column headings in Tables 3-3(9)

Symbol	Definition
T_b	Normal boiling point
$\Delta_v H$	Latent enthalpy of vaporization
S_b	Latent entropy of vaporization $\Delta_v H/T_b$
S_0	Reference entropy of vaporization (87.22 J mol^{-1} K^{-1})
$\delta P/\delta T$	Change in pressure with temperature
$U(T)$	Expanded uncertainty in T
$U(P)$	Expanded uncertainty in P
$U(\Delta_v H)$	Derived expanded uncertainty in $\Delta_v H$

3.3.3. References for Heats of Vaporization and Fusion

Reference	Source
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[2022TWE] This work estimate

4. Heats of Combustion and Formation

4.1. Overview

In this section, we present compiled, evaluated, and recommended standard state (T = 298.15 K) heats (enthalpies) of combustion and formation for hydrocarbons, substituted hydrocarbons, and a few other compounds of physical, chemical, and engineering interest. We provide over 1500 values for enthalpies of combustion and formation in the gas (about 700), liquid (about 750), and solid (about 90) phases for about 270 compounds taken from about 550 different sources. The enthalpies of combustion and formation were determined using a variety of methods, mainly combustion calorimetry, heats of hydrogenation, and heats of hydrolysis. The values provided here were taken from the literature, from the NIST Chemistry WebBook,[2021LIN], and the NIST TRC Thermodata Engine (TDE).[2021DIK] The recommended values of enthalpies of combustion and formation provided here were selected from reliable original sources (not weighted averages).

All the compiled values are contained in Table 4.8, while the selected recommended values are presented in Table 4.9. As a companion to the recommended combustion values in Table 4.9, we provide in Table 4.10 both "gross" and "net" heats of combustion, where "gross" are the heats of combustion where the products are at standard state (298.15 K and 1 bar) where water is in the liquid phase, while "net" are the heats of combustion where the products are all gaseous. For example, for combustion of chlorinated hydrocarbons the gross heat of combustion is where H_2O is liquid and HCl is in an aqueous solution, while the net heat of combustion is where both H_2O and HCl are in the gas phase. In the uncertainty column "unc", we provide the uncertainty as provided in the original – in many cases, the workers did not identify whether the uncertainties were 1σ or 2σ. On the other hand, all of our recommended values are 2σ.

Most of the enthalpies of combustion/formation in these tables are derived from heats of combustion (in the liquid or gas phase), although there are a fair number derived from heats of hydrogenation, hydrolysis, or other chemical reactions. In the cases where the original source data is not from combustion, the heat of combustion is derived from the heats of formation. The reverse is also true – heats of formation derived from heats of combustion. For many compounds, the "best" (selected) value of enthalpy of vaporization (or fusion) is used to compute enthalpies of formation in one phase from another phase, *i.e.*, $\Delta_f H$(gas) = $\Delta_f H$(liq) + $\Delta_v H$ or $\Delta_f H$(liq) = $\Delta_f H$(sol) + $\Delta_{fus} H$.

Tables 4-1, 4-2, 4-3, 4-4, and 4-5 provide descriptions of the notations used in the tables, while Tables 4-6 and 4-7 (and text in Sec. 4.2. Heats of Dilution) provide information about heats of dilution for aqueous solutions of HF, HCl, HBr, H_2SO_4 (sulfuric acid), and H_3BO_3 (boric acid).

In the tables in this section, as with other sections, the compounds are arranged first by primary and secondary chemical class and then by chemical formula.

Primary and Secondary Chemical Classes

1. **Small Molecules**
2. **Hydrogen/Oxygen**
   a. Nitrogen/Hydrogen
   b. Nitrogen/Oxygen
   c. Sulfur/Hydrogen/Oxygen
   d. Boron/Hydrogen/Oxygen
   e. Hydrogen Halides
3. **Hydrocarbons**
   a. Carbon
   b. Alkenes
   c. Alkadienes
   d. Alkynes
   e. Alkenynes
   f. Alkadiynes
   g. Cycloalkanes
   h. Cycloalkenes
   i. Cycloalkadienes
   j. Bicycloalkanes
4. **Aromatic Hydrocarbons**
   a. Alkylbenzenes
   b. Alkenylbenzenes
   c. Benzocycloalkanes
   d. Benzocycloalkenes
   e. Alkylnapthalenes
   f. Polycyclic Aromatics
5. **Oxidized Hydrocarbons**
   a. Carbon Oxides
   b. Alkanols
   c. Glycols
   d. Sugars
   e. Phenols
   f. Alkyl ethers
   g. Aldehydes
   h. Alkenals
   i. Ketones
   j. Carboxylic Acids
   k. Alkyl Esters
   l. Alkenyl Esters
   m. Alkanoic Anhydrides
   n. Oxacycloalkanes
   o. Oxacycloalkadienes
   p. Oxacycloketones
   q. Dioxanes and Trioxanes
   r. Furandione and D-Camphor
   s. Aromatic Alcohols
   t. Aromatic Aldehydes and Acids
6. **Nitrogen-Substituted Hydrocarbons**
   a. Hydrogen Cyanides
   b. Alkylamines
   c. Cycloalkylamines
   d. Azacycloalkanes
   e. Methenamines
   f. Azacycloalkadienes
   g. Alkanenitriles
   h. Alkenenitriles
   i. Cyanogens
   j. Alkylhydrazines
   k. Melamines
   l. Pyridines
   m. Anilines
   n. Oxidized Amines
   o. Alkyl Nitrates and Nitroalkanes
   p. Isocyanates
   q. Nitro Aromatics
7. **Sulfur-Substituted Hydrocarbons**
   a. Alkanethiols
   b. Alkyl Sulfides
   c. Thiacycloalkanes
   d. Thiacycloalkenes
   e. Aromatic Thiols
   f. Alkyl Sulfoxides
8. **Halogen-Substituted Hydrocarbons**
   a. Fluoroalkanes
   b. Fluoroalkenes
   c. Chloroalkanes
   d. Chloroalkenes
   e. Chloroacetylenes
   f. Chloroaromatics
   g. Bromoalkanes
   h. Bromoalkenes
   i. Iodoalkanes
   j. Chlorofluoromethanes
   k. Chlorofluoroethanes
   l. Chlorofluoroalkenes
   m. Bromofluoroalkanes
   n. Bromochloroalkanes
   o. Bromochlorofluoroalkanes
   p. Carbonyl Halides
   q. Chlorophenols
9. **Siloxanes**

Table 4-11). Notations for column headings

Symbol	Description
Formula	molecular formula
Compound	chemical name
T_{trs}	transition temperature: boiling (l), melting (s), or sublimation (s) note: normal boiling and melting points at 1 atm
Ph	phase below the transition temperature
SEL	selected (recommended) value
$\Delta_c H$	enthalpy of combustion at 298.15 K with H_2O (liq)
$\Delta_f H$	enthalpy of formation at 298.15 K with H_2O (liq)
$\Delta_{trs} H$	enthalpy of vaporization, fusion, or sublimation at 298.15 K
u	reported uncertainty in enthalpy of combustion, formation, or transition note: this is the reported uncertainty, not the standard uncertainty
M	method (see Table 4-4)
R	Denotes revised value (see notes below)
Ref	reference

Table 4-12). Notations for phase column

Notation	Phase
s	solid
l	liquid
g	gas
aq	aqueous solution
sl	denotes melting point
ls	denotes sublimation point
lg	denotes boiling point
s(d)	denotes decomposition temperature of a solid

Table 4-13). Notations for selected values column

)

SEL	Description
SEL	selected value at standard state (298 K, 1 atm)
SEL1	selected value in phase 1 (not standard state)
SEL2	selected value in another phase 2 (not standard state)
u	denotes a very uncertain value

Table 4-1(4). Notations for methods column

Method	Definition
BDE	from bond dissociation energy
Br2	from reaction involving Br_2
C	from enthalpy of combustion
C(l)	from enthalpy of combusiton of liquid
cal	calorimetry
CaO2	from reaction involving CaO_2H_2
CBS	calculated value using complete basis set method
CC	calculated value using coupled cluster methd
Cl2	from reaction using Cl_2
D	derived from enthalpy of decomposition
def	by definition
DfusH	computed using reference value for enthalpy of fusion
DsubH	computed using reference value for enthalpy of sublimation
DvH	computed using reference value for enthalpy of vaporization
E	derived using equilbrium reaction
est	estimated value
f	reference value for enthalpy of fusion
f(est)	derived using estimated enthalpy of fusion
F2	from reaction using F_2

Method	Definition
G3B3	calculated value using G3B3 method
H2	from enthalpy of hydrogenation
H2O	from enthalpy of hydrolysis
HBr	from reaction using HBr
HCl	from reaction using HCl
Hde	from enthalpy of dehydrogenation
I2	from heats of iodination
ion	from heat of ion/molecule reaction
K	from enthalpy of combustion using K
LiAl	from enthalpy of reduction using Lithium aluminum hydride
LiB	from enthalpy of reduction using Lithium triethylborohydride
Na	from enthalpy of combustion using Na
NF3	from reaction using NF_3
QM	calculated value using quantum chemistry
R	review value
s	reference value for enthalpy of sublimation
TN	calculated using a thermochemical network
v	reference value for enthalpy of vaporization

Table 4-1(5). Notations for revised values contained in column "R"

This table contains notation associated with the method to compute enthalpies of formation and combustion. In the first 4 cases (a through d), the values were recalculated by later work. In last 5 cases (e through k), the original aqueous dilutions that were measured or assumed for H_2SO_4 and HF are provided. The heats of formation of the aqueous dilutions are provided in Tables 4-8 and 4-9.

Note	Description
a	recalculated by 1965COX
b	recalculated by 1970COX
c	recalculated by 2002MAN
d	recalculated by 2019PAU
e	H_2SO_4 (aq, 30 H_2O)
f	H_2SO_4 (aq, 45 H_2O)
g	H_2SO_4 (aq, 115 H_2O)
j	HF (aq, 22 H_2O)
k	HF (aq, 23 H_2O)

4.2. Heats of Dilution

Where the standard state for a product of combustion is an aqueous solution, we have computed heats of combustion and formation employing standard enthalpies of dilution for HF, HCl, HBr, sulfuric acid (H_2SO_4), and boric acid (H_3BO_3).

Aqueous Dilutions for HCl

The notation, for example, HF (aq, 20 H_2O) means a dilution of one part HF in 20 parts H_2O and the reaction for the combustion of difluoromethane (gas) can be written equivalently as

$$CH_2F_2 + O_2 \rightarrow CO_2 + 2\ HF\ (aq, 20\ H_2O), \text{ or}$$
$$CH_2F_2 + O_2 + 40\ H_2O \rightarrow CO_2 + 2\ [HF{\cdot}20\ H_2O]$$

Various workers have used different heats of dilution for HF in aqueous soluutions for combustion of fluorinated hydrocarbons depending on the calculated final concentrations of HF in water (or assumed concentrations). This impacts the enthalpies of formation derived from the enthalpies of combustion by on the order of 0.15 kJ mol^{-1} with final dilutions ranging from HF (aq, 10 H_2O) to HF (aq, 50 H_2O). There are other factors that also impact the derived enthalpies of formation by as much as about 30 kJ mol^{-1} as discussed by Cox et al [1965COX] and Paulechka and Kazakov [2019PAU]. The following table shows dilutions determined (or assumed) for a set of fluorinated hydrocarbons. We utilize the enthalpy of formation (-321.05±0.16) kJ mol^{-1} from Ruscic and Bross [2021RUS] for HF (aq, 20 H_2O) to derive enthalpies of combustion and formation.

Table 4-2(1). Compounds and references for aqueous dilutions for HF

Compound	HF Dilution	Reference
CH_2F_2	23 H_2O	2021RUS
CH_2F_2	22 H_2O	1958NEU
CHF_3	24 H_2O	1958NEU
CF_4	20 H_2O	1965COX
CF_4	20 H_2O	1967DOM
CF_4	10 H_2O	1965DOM
CF_4	10 H_2O	1956GOO
CF_4	10 H_2O	1968GRE
CF_4	10 H_2O	1955SCO
CH_3CHF_2	20 H_2O	1968KOL
CH_3CF_3	27 H_2O	1965KOL
CH_2CHF	40 H_2O	1970KOL
CH_2CF_2	50 H_2O	1956NEU
CH_2CF_2	30 H_2O	1962KOL
$CHFCF_2$	30 H_2O	1962KOL

Aqueous Dilutions for HCl

Most workers have used a standard dilution for HCl of HCl (aq, 600 H_2O) to compute enthalpies for formation from enthalpies of combustion for the chlorinated hydrocarbons. This has been in standard since the work of Smith et al [1953SMI] based on the heats of dilution contained in NBS Circular 500.[1952ROS] The enthalpy of formation for HCl (aq, 600 H_2O) is (-166.452±0.024) kJ mol^{-1}.[2021RUS] We have used this value to compute enthalpies of combustion for enthalpies of formation. The following table lists a number of chlorinated hydrocarbons and references for the enthalpy of combustion measurements. Overall, for HCl, we consider the uncertainty due to dilution is about 0.3 kJ mol^{-1} per HCl.

Table 4-2(2). Compounds and references for aqueous dilution for HCl

Compound	HCl Dilution	Reference
CH_3Cl	600 H_2O	1971FLE
CH_2Cl_2	600 H_2O	1969HU
$CHCl_3$	600 H_2O	1969HU
CCl_4	600 H_2O	1969HU
CH_3CH_2Cl	600 H_2O	1971FLE
CH_3CH_2Cl	600 H_2O	1972HU
CH_2ClCH_2Cl	600 H_2O	1958SIN
CH_3CCl_3	600 H_2O	1972HU
CH_2ClCCl_3	600 H_2O	1978GUN
CH_2CHCl	600 H_2O	1964JOS
$CH2CCl_2$	600 H_2O	1971MAN
CH_2CCl_2	600 H_2O	1958SIN
$CHClCCl_2$	600 H_2O	1985PAP

Aqueous Dilutions for HBr, H_2SO_4, and H_3BO_3

HBr (aq, 600 H_2O) is considered the standard dilution for hydrogen bromide; we have utilized the enthalpy of formation of (-120.11±0.15) kJ mol^{-1} taken from Ruscic et al [2021RUS]. H_2SO_4 (aq, 115 H_2O) is considered the standard dilution for sulfuric acid; we have utilized the enthalpy of formation of (-887.81±0.25) kJ mol^{-1} taken from Wagman et al.[1982WAG]. H_3BO_3 (aq, 500 H_2O) is considered the standard dilution for boric acid; we have utilized the enthalpy of formation taken of (-1069.89±0.13) kJ mol^{-1} from Smisko and Mason.[1950SMI]

4.3. Heats of Combustion, Formation, and Transition (Compiled)

The following Table 4-3 contains all the compiled heats of combustion $\Delta_c H$, formation $\Delta_f H$, and transition $\Delta_f H$ for many compounds at standard state, while Table 4-4 contains only the selected/recommended values. The compounds are listed first by primary and secondary compound class, and then by molecular formula. The notations used for Ph (phase), SEL (selected), M (method), and R (revised) are given in Tables 4-1(2), 4-1(3), 4-1(4), and 4-1(5).

Table 4-14. Heats of Combustion, Formation, and Transition

Formula	Compound	T_{trs} [K]	Ph	SEL	$\Delta_c H$	*u*	$\Delta_f H$	*u*	$\Delta_{trs} H$	*u*	M	R	Ref
					kJ mol^{-1}								
SMALL MOLECULES													
Hydrogen/Oxygen													
H_2	hydrogen	20.37	g	SEL	-285.826	0.000	0.000	0.000			def		def
O_2	oxygen	90.19	g	SEL	0.000	0.000	0.000	0.000			def		def
H_2O_2	hydrogen peroxide	426.40	l	SEL	-98.48	0.79	-187.35	0.79	51.89	0.79	TN		2021RUS
		426.40	g	SEL1	-150.368	0.068	-135.458	0.063			TN		2021RUS
		272.74	s	SEL2	-86.26	0.79	-199.56	0.79	12.22	0.03	DfusH		1955GIG
		426.40	g		-150.6	2.7	-135.2	2.7			R		2019DIK
		426.40	g		-150.32	0.06	-135.51	0.05			BDE		1992LUO
		426.40	g		-149.1	0.4	-136.7	0.4			BDE		1988LIT
		426.40	g		-149.9	0.2	-135.9	0.2			D		1955GIG
		426.40	g		-98.49	0.17	-187.34	0.17			C		1951FOL
		426.40	l		-98.24	0.13	-187.59	0.13			C		1930ROT
		426.40	l		-98.198	0.084	-187.628	0.084			C		1929MAT
		426.40	lg						51.63				1955GIG
		272.74	sl	SEL					12.22	0.03	f		1951FOL
H_2O	water	373.12	l	SEL	0.000	0.037	-285.826	0.026	44.00	0.22	TN		2021RUS
		373.12	g	SEL1	-43.994	0.037	-241.832	0.026			TN		2021RUS
		273.153	s	SEL2	6.913	0.037	-292.739	0.026	6.91		TN		2021RUS
		373.12	g		-44.01	0.05	-241.82	0.04			R		2019DIK
		373.12	g		-44.00	0.05	-241.83	0.04			R		1984COX

		373.12	g		-43.99	0.22	-241.83	0.22			D	1968KIN
		373.12	g		-44.04	0.05	-241.79	0.04			D	1939ROS
		373.12	l		-0.06	0.19	-285.77	0.19	43.95	0.19	R	2019DIK
		373.12	l		0.00	0.05	-285.83	0.04			R	1984COX
		273.153	sg						50.88			2006REI
Nitrogen/Hydrogen												
N_2	nitrogen	77.36	g	SEL	0.000	0.000	0.000	0.000			def	
H_3N	ammonia	239.82	g	SEL	-383.181	0.029	-45.558	0.029			TN	2021RUS
		239.82	l	SEL1	-363.32	0.11	-65.42	0.11			DvH	2021RUS
		239.82	lg	SEL					19.87	0.10	v	2019DIK
ClH_4NO_4	ammonium perchlorate	403.15	s(d)	SEL	-442.33	0.17	-295.77	0.17				1998CHA
		403.15	s(d)		-452.3		-285.8	1.3				2019DIK
H_4N_2	hydrazine	386.65	l	SEL	-622.34		50.69	0.18	-336.51	1.00		2021RUS
		386.65	g	SEL1	-669.22		97.6	1.0				2021RUS
		386.65	g		-667.60		95.95	0.63				2019DIK
		386.65	g		-664.7		93.1					1939HUG
		386.65	l		-621.80		50.15	0.32	45.80	0.54		2019DIK
		386.65	l		-622.3		50.6		42.47			1939HUG
Hydrogen Halides												
FH	hydrogen fluoride	292.7	g	SEL	na		-272.721	0.048			TN	2021RUS
		292.7	l	SEL1	na		-302.41	0.16			TN	2021RUS
		292.7	g		na		-273.3	0.7			R	1984COX
	hydrogen fluoride (aq)	293.15	aq		na		-334.50	0.16			TN	2021RUS
	hydrogen fluoride (aq, 10 H_2O)	293.15	aq		na		-320.88	0.16			TN	2021RUS
	hydrogen fluoride (aq, 20 H_2O)	293.15	aq	SEL	na		-321.05	0.16			TN	2021RUS
	hydrogen fluoride (aq, 22 H_2O)	293.15	aq		na		-321.06	0.16			TN	2021RUS
	hydrogen fluoride (aq, 23 H_2O)	293.15	aq		na		-321.07	0.16			TN	2021RUS
	hydrogen fluoride (aq, 24 H_2O)	293.15	aq		na		-321.08	0.16			TN	2021RUS
	hydrogen fluoride (aq, 27 H_2O)	293.15	aq		na		-321.10	0.16			TN	2021RUS
	hydrogen fluoride (aq, 30 H_2O)	293.15	aq		na		-321.11	0.16			TN	2021RUS
	hydrogen fluoride (aq, 40 H_2O)	293.15	aq		na		-321.14	0.16			TN	2021RUS
	hydrogen fluoride (aq, 50 H_2O)	293.15	aq		na		-321.16	0.16			TN	2021RUS
	hydrogen fluoride (aq, 60 H_2O)	293.15	aq		na		-321.18	0.16			TN	2021RUS
ClH	hydrogen chloride	188.1	g	SEL	na		-92.173	0.006			TN	2021RUS
		188.1	g		na		-92.31	0.10			R	1984COX
	hydrogen chloride (aq)	293.15	aq		na		-166.992	0.023			TN	2021RUS
	hydrogen chloride (aq, 600 H_2O)	293.15	aq	SEL	na		-166.452	0.024			TN	2021RUS

BrH	hydrogen bromide	206.77	g	SEL	na		-36.29	0.16			R	1984COX
		206.77	g		na		-35.45	0.14			TN	2021RUS
	hydrogen bromide (aq)	293.15	aq		na		-120.59	0.15			TN	2021RUS
	hydrogen bromide (aq, 600 H_2O)	293.15	aq	SEL	na		-120.11	0.15			TN	2021RUS
Sulfur/Hydrogen/Oxygen												
H_2S	hydrogen sulfide	212.85	g	SEL	-867.21	0.5	-20.6	0.5			R	1984COX
		212.85	l	SEL1	-853.55	0.64	-34.27	0.64			DvH	1984COX
		212.85	lg	SEL					13.67	0.40	v	2019DIK
O_2S	sulfur dioxide	263.14	l	SEL	na		-320.5	1.0	23.67		R	1982WAG
		263.14	g	SEL1	na		-296.83	0.20			R	1982WAG
		263.14	g		na		-296.81	0.20			R	2019DIK
		263.14	lg						22.93	1.03	R	2019DIK
H_2O_4S	sulfuric acid	283.46	l	SEL1	na		-814.0	1.0			R	1982WAG
		283.46	g	SEL2	na		-735.1	1.0			R	1998CHA
	sulfuric acid (aq, 115 H_2O)	283.46	aq	SEL	na		-887.81	0.25			R	1982WAG
		283.46	aq		na	35.98	-888.01	0.29			H2O	1963MAN
		283.46	aq		na	1.17	-887.72	0.25			H2O	1960GOO
	sulfuric acid (aq, 30 H_2O)	283.46	aq		na		-885.98	0.25			R	1982WAG
	sulfuric acid (aq, 45 H_2O)	283.46	aq		na		-886.62	0.25			R	1982WAG
Boron Compounds												
BH_3O_3	boric acid	444.05	s	SEL	na		-1091.94	0.13			D	1950SMI
	boric acid (aq)	444.05	aq		na		-1069.26	0.13			H2O	1950SMI
	boric acid (aq, 500 H_2O)	444.05	aq	SEL	na		-1069.89	0.13			H2O	1950SMI
B_2H_6	diborane	180.59	g	SEL	-2175.76	1.17	36.0	1.2			D	1965GUN
		180.59	l	SEL1	-2174.75	1.17	35.0	1.2			DvH	1965GUN
		180.59	g		-2180.8	16.7	41	17			R	1998CHA
		180.59	g		-2175.34		35.56				R	1988RUS
		180.59	g		-2176.2		36.40				R	1982WAG
		180.59	g		-2175.1	2.3	35.3	2.3			D	1965GUN
		180.59	g		-2176.52	1.17	36.7	1.2			D	1965GUN
		180.59	g		-2177.11	0.63	37.33	0.63			H2O	1960GUN
		180.59	g		-2167.9	2.2	28.2	2.2			D	1958PRO
		180.59	l		-2166.9	2.2	27.2	2.2			D	1958PRO
		180.59	lg	SEL			36.8		1.01		v	1959PAR
B_2O_3	diboron trioxide	723.15	s	SEL	na		-1279.9	2.1				1959JOH
		2130	g	SEL1	na		-836.0	4.2				1963HIL
		2130	l	SEL2	na		-1259.3	1.3				1961NBS

	2130	g	na	-834	13				2011JAC
	2130	g	na	-834.2	8.4				1978SCH
	2130	g	na	-848.5	8.7			DsubH	1959JOH
	2130	g	na	-829.2	3.9				1957SCH
	2130	l	na	-1253.4	2.5				1998CHA
	723.15	s	na	-1271.9	2.1				1998CHA
	723.15	s	na	-1273.5	1.4				1984COX
	723.15	s	na	-1277.5	1.4				1961NBS
	723.15	s	na	-1278.2	1.9				1960GUN
	723.15	s	na	-1280.9	3.1				1959PRO
	723.15	sg				431.4	8.4		1963HIL

HYDROCARBONS												
Carbon												
C	diamond	4300	s	SEL1	-395.347	0.070	1.871	0.070			C	1966HAW
	graphite	4800	s	SEL	-393.476	0.025	0.000	0.025			def	1966HAW
		5000	g	SEL1	-1110.359	0.047	716.883	0.045			TN	2021RUS
Alkanes												
CH_4	methane	111.67	g	SEL	-890.602	0.050	-74.526	0.049			TN	2021RUS
		111.67	g		-890.52	0.36	-74.61	0.36			R	2019DIK
		111.67	g		-890.46	0.35	-74.67	0.35			C	2002YU
		111.67	g		-890.61	0.21	-74.52	0.21			C	2002DAL
		111.67	g		-890.53	0.30	-74.60	0.30			R	1989GUR
		111.67	g		-890.7	0.4	-74.4	0.4			C	1972PIT
		111.67	g		-890.35	0.30	-74.78	0.31			C	1945PRO
		111.67	g		-891.8	1.1	-73.3	1.1			C	1932ROT
		111.67	g		-890.16	0.30	-74.97	0.30			C	1931ROS
C_2H_6	ethane	184.57	g	SEL	-1560.39	0.13	-84.04	0.13			TN	2021RUS
		184.57	l	SEL1	-1555.58	1.03	-88.85	1.03			DvH	2021RUS
		184.57	g	SEL	-1560.34	0.99	-84.09	0.99	4.81	0.29	v	2019DIK
		184.57	g		-1560.4	0.4	-84.0	0.4			R	1989GUR
		184.57	g		-1560.70	0.30	-83.73	0.30			C	1972PIT
		184.57	g		-1559.90	0.49	-84.53	0.49			C	1945PRO
		184.57	g		-1559.84	0.46	-84.59	0.46			C	1934ROS
		184.57	lg						9.76		R	1985MAJ
C_3H_8	propane	231.04	g	SEL	-2218.66	0.16	-105.07	0.16			TN	2021RUS
		231.04	l	SEL1	-2203.31	0.26	-120.42	0.26			DvH	2021RUS
		231.04	g		-2219.28	1.10	-104.45	1.10			R	2019DIK
		231.04	g		-2219.2	0.5	-104.5	0.5			C	1972PIT
		231.04	g		-2219.93	0.54	-103.80	0.59			DvH	1945PRO
		231.04	g		-2219.9	0.5	-103.8	0.5			C	1934ROS
		231.04	g		-2206.6		-117.1				C	1918GUI
		231.04	l		-2204.49	1.12	-119.24	1.12	14.79	0.18	R	2019DIK
		231.04	lg						16.25		R	1985MAJ
		231.04	lg	SEL					15.4		v	1945PRO
C_4H_{10}	isobutane	261.40	g	SEL	-2868.41	0.30	-134.62	0.30			TN	2021RUS
		261.40	l	SEL1	-2848.95	0.37	-154.08	0.37			DvH	2021RUS
		261.40	g		-2868.1	1.5	-134.9	1.5			R	2019DIK
		261.40	g		-2869.00	0.59	-134.03	0.63			C	1972PIT

		261.40	g		-2867.60	0.46	-135.43	0.54			C	1951PRO
		261.40	l	SEL	-2848.6	1.7	-154.4	1.7	19.46	0.21	v	2019DIK
		261.40	lg						19.99		R	1985MAJ
	n-butane	272.66	g	SEL	-2877.28	0.24	-125.75	0.24			TN	2021RUS
		272.66	l	SEL1	-2854.88	0.69	-148.15	0.69			DvH	2021RUS
		272.66	g		-2876.7	1.5	-126.3	1.5			R	2019DIK
		272.66	g		-2877.50	0.63	-125.53	0.67			C	1972PIT
		272.66	g		-2876.20	0.67	-126.83	0.67			C	1951PRO
		272.66	g		-2878.34	0.63	-124.69	0.63			C	1934ROS
		272.66	l		-2856.33	1.16	-146.70	1.16	20.41	0.21	R	2019DIK
		272.66	lg	SEL					22.40		v	1971WIL
C_5H_{12}	isopentane	300.98	l	SEL	-3503.95	0.43	-178.39	0.43			TN	2021RUS
		300.98	g	SEL1	-3529.17	0.43	-153.17	0.43			TN	2021RUS
		300.98	g		-3528.69	0.92	-153.65	0.92			R	2019DIK
		300.98	g		-3528.66	0.59	-153.68	0.59			DvH	1970GOO
		300.98	g		-3528.40	0.92	-153.94	0.96			C	1967PIL
		300.98	g		-3528.60	0.63	-153.74	0.63			C	1939KNO
		300.98	g		-3527.6	3.5	-154.7	3.5			C	1936ROT
		300.98	l		-3503.89	0.97	-178.45	0.97	24.80	0.32	R	2019DIK
		300.98	l		-3504.40	0.84	-177.94	0.88	24.50		C	1979GOO
		300.98	l		-3503.30	0.75	-179.04	0.84	24.80		C	1945PRO
		300.98	lg	SEL					25.22		v	1985MAJ
		300.98	lg						24.80			1971WIL
		300.98	lg						24.84	0.13		1951SCO
		300.98	lg						25.00			1942SCH
	neopentane	282.65	l	SEL	-3492.56	0.39	-189.78	0.39	22.39	0.30	TN	2021RUS
		282.65	g	SEL1	-3514.95	0.39	-167.39	0.39			TN	2021RUS
		282.65	g		-3514.03	0.88	-168.30	0.88			R	2019DIK
		282.65	g		-3514.10	0.92	-168.24	0.96			C	1967PIL
		282.65	l		-3492.20	0.88	-190.14	0.88	21.84	0.06	R	2019DIK
		282.65	l		-3492.43	0.84	-189.91	0.59	22.38	0.59	C	1970GOO
		282.65	l		-3494.4	0.8	-187.9	1.0	22.20		C	1945PRO
		282.65	lg						22.39			1985MAJ
		282.65	lg						21.80			1981HOS2
		282.65	lg						21.85			1971WIL
	n-pentane	309.21	l	SEL	-3509.35	0.43	-172.99	0.43	26.74	0.20	TN	2021RUS
		309.21	g	SEL1	-3536.09	0.31	-146.25	0.31			TN	2021RUS

		309.21	g		-3535.27	0.73	-147.06	0.73			R	2019DIK
		309.21	g		-3535.54	0.59	-146.80	0.59			DvH	1979GOO
		309.21	g		-3535.4	1.0	-146.9	1.0			C	1967PIL
		309.21	g		-3536.60	0.88	-145.74	0.88			C	1934ROS
		309.21	l		-3508.90	0.72	-173.44	0.72	26.38	0.12	R	2019DIK
		309.21	l		-3509.04	0.46	-173.30	0.47	26.73	0.42	C	1970GOO
		309.21	l		-3509.50	0.59	-172.84	0.67	26.70		C	1945PRO
		309.21	l		-3509.16	0.75	-173.17	0.75			C	1944PRO
		309.21	lg						26.20			2010HOR
		309.21	lg						26.40			1994RUZ
		309.21	lg						26.75		R	1985MAJ
		309.21	lg						26.60	0.10		1984LAW
		309.21	lg						26.60	0.10		1982FUC
		309.21	lg						26.40			1981HOS
		309.21	lg						26.40			1971WIL
		309.21	lg						26.42			1947OSB
		309.21	lg						27.40			1945WIL
		309.21	lg						26.20			1940MES
C_6H_{14}	3-methylpentane	336.43	l	SEL	-4159.90	0.88	-201.74	0.96	30.30	0.10	C	1945PRO
		336.43	g	SEL1	-4190.2	1.0	-171.4	1.0			DvH	1945PRO
		336.43	g		-4189.5	1.9	-172.2	1.9			R	2019DIK
		336.43	l		-4159.2	1.9	-202.4	1.9	30.24	0.18	R	2019DIK
		336.43	lg						30.47		R	1985MAJ
		336.43	lg						30.30	0.10		1979MAJ
		336.43	lg						30.30			1971WIL
		336.43	lg						30.19	0.03		1966WAD
		336.43	lg	SEL					30.27	0.10	v	1947OSB
	isohexane	333.42	l	SEL	-4157.65	0.83	-203.99	0.83	30.11	0.20	TN	2021RUS
		333.42	g	SEL1	-4187.76	0.84	-173.88	0.84			TN	2021RUS
		333.42	g		-4186.8	2.0	-174.9	2.0			R	2019DIK
		333.42	l		-4157.0	1.9	-204.7	1.9	29.79	0.26	R	2019DIK
		333.42	l		-4157.3	1.0	-204.3	1.0	30.0		C	1945PRO
		333.42	lg						30.10		R	1985MAJ
		333.42	lg						29.90			1971WIL
		333.42	lg						29.89	0.10		1949WAD
		333.42	lg						24.86	0.10		1947OSB
	neohexane	322.89	l	SEL	-4148.50	0.88	-213.14	0.96	27.68	0.20	C	1945PRO

		322.89	g	SEL1	-4176.18	0.96	-185.46	0.96			DvH	1945PRO
		322.89	g		-4175.4	2.0	-186.3	2.0			R	2019DIK
		322.89	l		-4147.8	1.9	-213.8	1.9	27.56	0.34	R	2019DIK
		322.89	lg						27.93		R	1985MAJ
		322.89	lg						27.70			1971WIL
		322.89	lg	SEL					27.68		v	1947OSB
	n-hexane	341.87	l	SEL	-4163.04	0.34	-198.60	0.34	31.71	0.20	TN	2021RUS
		341.87	g	SEL1	-4194.75	0.39	-166.89	0.39			TN	2021RUS
		341.87	g		-4194.52	0.93	-167.12	0.93			R	2019DIK
		341.87	l		-4163.02	0.91	-198.61	0.91	31.50	0.19	R	2019DIK
		341.87	l		-4163.20	0.67	-198.44	0.67	31.6		C	1969GOO
		341.87	l		-4163.10	0.54	-198.54	0.79	31.6		C	1945PRO
		341.87	l		-4163.00	0.71	-198.64	0.71			C	1944ROS
		341.87	l		-4163.7	1.4	-197.9	1.4			C	1937JES
		341.87	lg						31.40	0.20		2007PAS
		341.87	lg						31.50	0.10		1996VAR
		341.87	lg						31.50			1994RUZ
		341.87	lg						32.10			1992GRA
		341.87	lg						31.73		R	1985MAJ
		341.87	lg						31.60	0.10		1979MAJ
		341.87	lg						31.55			1971WIL
		341.87	lg						29.96			1957GLA
		341.87	lg						31.54	0.10		1947OSB
		341.87	lg						31.00	0.20		1943LEM
C_7H_{16}	n-heptane	371.55	l	SEL	-4816.83	0.46	-224.11	0.46	36.65	0.20	TN	2021RUS
		371.55	g	SEL1	-4853.48	0.46	-187.46	0.46			TN	2021RUS
		371.55	g		-4853.4	1.3	-187.6	1.3			R	2019DIK
		371.55	l		-4816.8	1.3	-224.2	1.3	36.59	0.33	R	2019DIK
		371.55	l		-4825.0		-215.9				C	1973DEL
		371.55	l		-4818.7		-222.2				C	1957SKU
		371.55	l		-4816.91	0.63	-224.03	0.79	36.6		C	1945PRO
		371.55	l		-4817.16	0.88	-223.78	0.88	35.98		C	1944PRO
		371.55	l		-4810.3		-230.6				C	1941JON
		371.55	l		-4815.0	1.0	-225.9	1.3	36.6		C	1941DAV
		371.55	l		-4817.0	1.5	-223.9	1.5			C	1937JES
		371.55	lg						36.60			1994RUZ
		371.55	lg						36.66		R	1985MAJ

		371.55	lg						36.60	0.10		1979MAJ
		371.55	lg						36.90			1979JAK
		371.55	lg						36.55			1971WIL
		371.55	lg						36.54			1947OSB
		371.55	lg						32.01	0.17		1926MAT
C_8H_{18}	n-octane	398.79	l	SEL	-5470.63	0.55	-249.61	0.55	41.53	0.20	TN	2021RUS
		398.79	g	SEL1	-5512.16	0.54	-208.08	0.54			TN	2021RUS
		398.79	g		-5511.61	1.09	-208.63	1.09			R	2019DIK
		398.79	l		-5470.07	1.05	-250.17	1.05	41.54	0.27	R	2019DIK
		398.79	l		-5470.3	1.6	-249.9	1.8	41.6		C	1972GOO
		398.79	l		-5470.10	0.67	-250.14	0.84	41.6		C	1945PRO
		398.79	l		-5466.6		-253.6				C	1937JES
		398.79	l		-5471.8	5.4	-248.4	5.4			C	1933BAN
		398.79	lg						41.60			1994RUZ
		398.79	lg						41.5		R	1985MAJ
		398.79	lg						41.50	0.10		1981HOS2
		398.79	lg						41.50	0.10		1979MAJ
		398.79	lg						41.5			1971WIL
		398.79	lg						41.59	0.08		1966WAD2
		398.79	lg						41.59	0.08		1960WAD
		398.79	lg						41.48	0.20		1947OSB
		398.79	lg						33.97			1920FAJ
C_9H_{20}	n-nonane	423.91	l	SEL	-6124.85	0.50	-274.69	0.50	46.44	0.20	TN	2021RUS
		423.91	g	SEL1	-6171.29	0.51	-228.25	0.51			TN	2021RUS
		423.91	g		-6170.77	1.14	-228.77	1.14			R	2019DIK
		423.91	l		-6124.42	0.99	-275.13	0.99	46.36	0.55	R	2019DIK
		423.91	l		-6125.21	0.54	-274.70	0.54	46.4		C	1969GOO
		423.91	l		-6124.9	1.1	-274.6	1.1			C	1944PRO
		423.91	l		-6119.8		-279.7				C	1937JES
		423.91	lg						46.50	0.20		2007PAS
		423.91	lg						46.60	0.20		1996VAR
		423.91	lg						46.60			1994RUZ
		423.91	lg						46.43		R	1985MAJ
		423.91	lg						46.40			1971WIL
		423.91	lg						46.43			1947OSB
$C_{10}H_{22}$	n-decane	447.27	l	SEL	-6778.29	0.80	-300.56	0.80	51.39	0.20	TN	2021RUS
		447.27	g	SEL1	-6829.68	0.91	-249.17	0.91			TN	2021RUS

		447.27	g		-6829.4	2.7	-249.5	2.7			R	2019DIK
		447.27	l		-6777.8	2.6	-301.0	2.6	51.55	0.39	R	2019DIK
		447.27	l		-6778.3	0.9	-300.5	1.1	51.3		C	1945PRO
		447.27	l		-6778.6	1.5	-300.2	1.5	50.9		C	1944PRO
		447.27	l		-6774.2		-304.6				C	1937JES
		447.27	lg						51.1	3.9		2000NIC
		447.27	lg						50.9			1995CHI
		447.27	lg						51.40			1994RUZ
		447.27	lg						51.37	0.02		1989CHI
		447.27	lg						51.4		R	1985MAJ
		447.27	lg						51.40	0.10		1982FUR
		447.27	lg						51.38	0.12		1972IRV
		447.27	lg						51.40			1971WIL
		447.27	lg						51.36			1947OSB
$C_{16}H_{34}$	n-hexadecane	559.94	l	SEL	-10699.1	1.8	-455.6	2.0	81.40	0.40	C	1955FRA
		559.94	g	SEL1	-10780.5	1.8	-374.2	2.0			DvH	1955FRA
		559.94	g		-10777.9	2.9	-376.7	2.9			R	2019DIK
		559.94	l		-10697.0	2.5	-457.6	2.5	80.90	1.40	R	2019DIK
		559.94	l		-10699.1	4.1	-455.6	4.1	81.4		C	1939RIC
		559.94	lg						81.80	1.30		2000NIC
		559.94	lg	SEL					81.4		v	1995CHI
		559.94	lg						81.40			1994RUZ
		559.94	lg						81.4		R	1985MAJ
		559.94	lg						81.40	0.40		1972MOR
		559.94	lg						81.1			1971WIL
		559.94	lg						80.60	1.50		1949PAR
Alkenes												
C_2H_4	ethene	169.38	g	SEL	-1410.92	0.12	52.32	0.12			TN	2021RUS
		169.38	l	SEL1	-1402.48	0.17	43.88	0.17			DvH	2021RUS
		169.38	g		-1411.12	0.57	52.52	0.57			R	2019DIK
		169.38	g		-1411.0	0.5	52.4	0.5			R	1989GUR
		169.38	g		-1411.20	0.30	52.60	0.30			C	1937ROS
		169.38	l	SEL	-1402.7	2.7	44.1	2.7	8.44	0.13	v	2019DIK
C_3H_6	propene	225.53	g	SEL	-2057.79	0.20	19.88	0.19			TN	2021RUS
		225.53	l	SEL1	-2043.57	0.33	5.66	0.33			DvH	2021RUS
		225.53	g		-2056.5	2.5	18.6	2.5			R	2019DIK
		225.53	g		-2058.3		20.4				E	1969FUR

		225.53	g		-2057.80	1.10	19.89	1.10			C	1968WIB
		225.53	g		-2058.3		20.4				HBr	1950LAC
		225.53	g		-2057.7	0.6	19.8	0.6			C	1937ROS
		225.53	l	SEL	-2042.3	2.5	4.4	2.5	14.22	0.27	v	2019DIK
C_4H_8	1-butene	266.83	g	SEL	-2717.30	0.36	0.09	0.36			TN	2021RUS
		266.83	l	SEL1	-2697.20	0.45	-20.01	0.45			DvH	2021RUS
		266.83	g		-2716.65	1.03	-0.56	1.03			R	2019DIK
		266.83	g		-2716.80	0.75	-0.41	0.76			C	1951PRO
		266.83	l		-2696.3	2.0	-20.9	2.0	20.32	0.30	R	2019DIK
		266.83	lg						20.88		R	1985MAJ
		266.83	lg	SEL					20.1		v	1971WIL
	2-butene, (E)-	274.01	g	SEL	-2706.07	0.38	-11.14	0.38			TN	2021RUS
		274.01	l	SEL1	-2684.77	0.41	-32.44	0.41			DvH	2021RUS
		274.01	g		-2706.6	1.0	-10.6	1.0			C	2019PRO
		274.01	g		-2706.48	1.18	-10.73	1.18			R	2019DIK
		274.01	g		-2706.63	0.96	-10.58	0.96			C	1951PRO
		274.01	l		-2685.09	1.19	-32.12	1.19	21.39	0.16	R	2019DIK
		274.01	lg						21.97		R	1985MAJ
		274.01	lg	SEL					21.3		v	1971WIL
	2-butene, (Z)-	276.87	g	SEL	-2710.16	0.40	-7.05	0.40			TN	2021RUS
		276.87	l	SEL1	-2688.06	0.59	-29.15	0.59			DvH	2021RUS
		276.87	g		-2709.6	1.4	-7.6	1.4			R	2019DIK
		276.87	g		-2709.8	1.3	-7.4	1.3			C	1951PRO
		276.87	l		-2688.8	7.6	-28.4	7.6	20.80	0.19	R	2019DIK
		276.87	lg						22.70		R	1985MAJ
		276.87	lg	SEL					22.1		v	1971WIL
	isobutene	266.05	g	SEL	-2700.20	0.39	-17.01	0.39			TN	2021RUS
		266.05	l	SEL1	-2679.60	0.50	-37.61	0.49			DvH	2021RUS
		266.05	g		-2699.3	1.3	-17.9	1.3			R	2019DIK
		266.05	g		-2699.50	1.10	-17.71	1.10			C	1951PRO
		266.05	l		-2677.8	7.2	-39.4	7.2	21.50	0.30	R	2019DIK
		266.05	lg	SEL					20.60		v	1971WIL
C_5H_8	2-Methyl-1,3-butadiene	307.19	l	SEL	-3159.50	0.72	48.82	0.72			DvH	2021RUS
		307.19	g	SEL1	-3186.28	0.67	75.60	0.67			TN	2021RUS
		307.19	g		-3186.4	2.1	75.8	2.1			R	2019DIK
		307.19	g		-3186.6	1.0	75.9	1.0			C	1955FRA
		307.19	l		-3160.2	2.1	49.5	2.1	26.22	0.22	R	2019DIK

		307.19	l		-3158.2	1.6	47.5	1.6			C	1938JES
		307.19	lg						26.40			1971WIL
		307.19	lg	SEL					26.78	0.25	v	1971ROG
C_5H_{10}	1-pentene	303.12	l	SEL	-3349.72	0.64	-46.79	0.64			C	1979GOO
		303.12	g	SEL1	-3375.22	0.67	-21.29	0.67			DvH	1979GOO
		303.12	g		-3374.93	0.93	-21.58	0.93			R	2019DIK
		303.12	l		-3349.5	0.8	-47.0	0.8	25.42	0.47	R	2019DIK
		303.12	l		-3349.57	0.43	-46.94	0.42			H2O	1984WIB
		303.12	l		-3349.6	2.5	-46.9	2.5			H2	1984MOL
		303.12	l		-3348.0	1.9	-48.5	1.9			H2	1984MOL
		303.12	l		-3345.6	2.5	-50.9	2.5			H2	1974ROG
		303.12	l		-3342.0	1.2	-54.5	1.2			H2	1971ROG
		303.12	lg						29.82		R	1985MAJ
		303.12	lg	SEL					25.5		v	1971WIL
		303.12	lg						25.50	0.10		1949SCO
	2-methyl-1-butene	304.30	l	SEL	-3335.74	0.84	-60.77	0.84			C	1979GOO
		304.30	g	SEL1	-3361.64	0.86	-34.87	0.86			DvH	1979GOO
		304.30	g		-3361.38	0.96	-35.13	0.96			R	2019DIK
		304.30	g		-3361.41	0.84	-35.10	0.84			H2O	1991WIB
		304.30	l		-3335.53	0.93	-60.98	0.93	25.85	0.26	R	2019DIK
		304.30	lg						26.19		R	1985MAJ
		304.30	lg	SEL					25.9		v	1971WIL
		304.30	lg						25.90	0.10		1949SCO
	2-pentene, (E)-	309.51	l	SEL	-3338.71	0.76	-57.80	0.76			C	1979GOO
		309.51	g	SEL1	-3365.4	0.8	-31.1	0.8			DvH	1979GOO
		309.51	g		-3365.2	1.4	-31.3	1.4			R	2019DIK
		309.51	g		-3364.87	0.45	-31.64	0.45			H2O	1984WIB
		309.51	g		-3363.4	1.3	-33.1	1.3			E	1966EGG
		309.51	l		-3338.5	1.3	-58.0	1.3	26.67	0.63	R	2019DIK
		309.51	l		-3338.27	0.42	-58.24	0.42			H2O	1984WIB
		309.51	l		-3336.8	1.0	-59.7	1.0			E	1966EGG
		309.51	l		-3335.9	0.4	-60.6	0.4			C	1946COO
		309.51	lg	SEL					26.7		v	1971WIL
	2-pentene, (Z)-	310.09	l	SEL	-3343.21	0.62	-53.30	0.62			C	1979GOO
		310.09	g	SEL1	-3370.0	0.7	-26.5	0.7			DvH	1979GOO
		310.09	g		-3369.80	0.79	-26.71	0.79			R	2019DIK
		310.09	g		-3368.5	0.8	-28.0	0.8			E	1966EGG

		310.09	l		-3343.00	0.77	-53.51	0.77	26.80	0.19	R		2019DIK
		310.09	l		-3343.16	0.43	-53.35	0.42			H2O		1984WIB
		310.09	l		-3336.66	0.30	-59.85	0.29			C		1946COO
		310.09	lg	SEL					26.8		v		1971WIL
	3-methyl-1-butene	293.21	g	SEL	-3369.00	0.68	-27.51	0.68			DvH		1979GOO
		293.21	l	SEL1	-3345.10	0.62	-51.41	0.62			C		1979GOO
		293.21	g		-3368.59	0.84	-27.92	0.84			R		2019DIK
		293.21	l		-3344.88	0.79	-51.63	0.79	23.71	0.29	R		2019DIK
		293.21	lg	SEL					23.9		v		1971WIL
C_6H_{12}	1-hexene	336.64	l	SEL	-4003.1	1.2	-72.7	1.2			H2		1984MOL
		336.64	g	SEL1	-4033.7	1.2	-42.1	1.2			DvH		1984MOL
		336.64	l		-4002.7	2.7	-73.2	2.7	-30.55	0.20	R		2019DIK
		336.64	l		-4003.5	1.2	-72.3	1.2			H2O		1981WIB
		336.64	l		-4003.8	0.8	-72.0	0.8			H2		1979ROG
		336.64	l		-4000.4	1.0	-75.4	1.0			H2		1975ROG
		336.64	l		-4003.7	1.2	-72.1	1.2			H2		1974ROG
		336.64	l		-4002.2	1.5	-73.6	1.5			H2		1970BRE
		336.64	l		-4003.7	1.0	-72.1	1.0			H2		1959SKI
		336.64	l		-4003.1	2.1	-72.7	2.1			H2		1957FLI
		336.64	lg	SEL					30.60		v		1971WIL
		336.64	lg						30.60				1956CAM
C_7H_{14}	1-heptene	366.71	l	SEL	-4657.41	0.63	-97.70	0.63			H2O		1984WIB
		366.71	g	SEL1	-4693.1	0.7	-62.0	0.7			DvH		1984WIB
		366.71	g		-4691.3	4.8	-63.8	4.8			R		2019DIK
		366.71	l		-4655.7	4.8	-99.4	4.8	35.59	0.21	R		2019DIK
		366.71	l		-4657.0	0.8	-98.1	1.2			C		1976GOO
		366.71	l		-4658.3	1.2	-96.8	1.2	36.07		C	b	1961ROC
		366.71	l		-4650.98	0.79	-104.13	0.79			C		1947COO
		366.71	lg	SEL					35.7		v		1971WIL
C_8H_{16}	1-octene	394.43	l	SEL	-5312.9	1.2	-121.5	1.2			C		1961ROC
		394.43	g	SEL1	-5353.5	1.2	-80.9	1.2			DvH		1961ROC
		394.43	g		-5353.1	1.7	-81.4	1.7			R		2019DIK
		394.43	g		-5351.5		-82.9				H2		1970BRE
		394.43	l		-5312.6	1.6	-121.8	1.6	40.44	0.54	R		2019DIK
		394.43	lg	SEL					40.60		v		1995CHI
		394.43	lg						40.44		R		1985MAJ
		394.43	lg						40.27	0.20			1977MAN

		394.43	lg						40.27	0.20		1977MAN
		394.43	lg						38.0			1971WIL
Alkadienes												
C_3H_4	allene	238.65	g	SEL	-1941.86	0.24	189.78	0.24			TN	2021RUS
		238.65	l	SEL1	-1925.30	0.69	173.22	0.69			DvH	2021RUS
		238.65	g		-1947.9	4.8	195.8	4.8			R	2019DIK
		238.65	l	SEL	-1931.3	4.8	179.3	4.8	16.56	0.65	v	2019DIK
C_4H_6	1,2-butadiene	284.06	g	SEL	-2593.79	0.46	162.41	0.46	23.68	0.30	TN	2021RUS
		284.06	l	SEL1	-2570.11	0.66	138.73	0.66			TN	2021RUS
		284.06	g		-2593.64	0.89	162.26	0.89			R	2019DIK
		284.06	g		-2593.80	0.54	162.42	0.54			C	1951PRO
		284.06	g		-2597.0	1.2	165.6	1.2			C	1949PRO
		284.06	l		-2570.36	0.92	138.98	0.92	23.28	0.22	R	2019DIK
		284.06	lg						23.68		R	1985MAJ
		284.06	lg						23.90			1971WIL
	1,3-butadiene	268.44	g	SEL	-2542.28	0.33	110.90	0.33			TN	2021RUS
		268.44	l	SEL1	-2521.18	0.43	89.80	0.43			DvH	2021RUS
		268.44	l	u	-2523	7	92	7	20.74	0.28	R	2019DIK
		268.44	g		-2540.21	1.03	108.83	1.03			R	2019DIK
		268.44	g		-2540.40	0.96	109.02	0.96			C	1951PRO
		268.44	l		-2522.10	0.96	87.62	0.96	21.40		C	1945PRO
		268.44	lg						21.47		R	1985MAJ
		268.44	lg	SEL					21.1		v	1971WIL
C_5H_8	1,2-pentadiene	318.80	l	SEL	-3222.90	0.69	112.22	0.69			DvH	1955FRA
		318.80	g	SEL1	-3251.60	0.67	140.92	0.67			C	1955FRA
		318.80	g		-3251.4	1.5	140.7	1.5			R	2019DIK
		318.80	l		-3223.0	1.5	112.3	1.5	28.41	0.17	R	2019DIK
		318.80	lg	SEL					28.7		v	1971WIL
	1,3-pentadiene	314.90	lg						27.78	1.19	R	2019DIK
	1,3-pentadiene, (E)-	315.32	l	SEL	-3158.90	0.78	48.22	0.78			DvH	1955FRA
		315.32	g	SEL1	-3186.70	0.67	76.02	0.67			C	1955FRA
		315.32	g		-3193.4	3.7	82.7	3.7			R	2012KRO
		315.32	l		-3165.8	3.8	55.1	3.8	27.6		R	2012KRO
		315.32	lg	SEL					27.8		v	1971WIL
	1,3-pentadiene, (Z)-	317.18	l	SEL	-3165.3	1.4	54.6	1.4			DvH	1955FRA
		317.18	g	SEL1	-3193.60	0.92	82.92	0.92			C	1955FRA
		317.18	lg	SEL					28.30	0.40	v	1971WIL

	1,4-pentadiene	299.12	g	SEL	-3217.2	1.3	106.5	1.3			C	1955FRA
		299.12	l	SEL1	-3192.0	1.3	81.3	1.3	25.20	0.20	DvH	1955FRA
		299.12	g		-3217.1	2.6	106.4	2.6			R	2019DIK
		299.12	l		-3191.9	2.7	81.3	2.7	25.13	0.21	R	2019DIK
		299.12	lg	SEL					25.2		v	1971WIL
Alkynes												
C_2H_2	acetylene	188.41	g	SEL	-1301.06	0.13	228.28	0.13			TN	2021RUS
		188.41	l	SEL1	-1293.7	4.4	220.9	4.4			DvH	2021RUS
		188.41	g		-1299.1	1.6	226.4	1.6			R	2019DIK
		188.41	g		-1300.2	0.8	227.4	0.8			R	1989GUR
		188.41	g		-1299.48	0.79	226.70	0.79			E	1945WAG
		188.41	l	SEL	-1291.8	4.7	219.0	4.7	7.4	4.4	v	2019DIK
C_3H_4	propyne	249.80	g	SEL	-1937.72	0.22	185.64	0.22			TN	2021RUS
		249.80	l	SEL1	-1918.14	0.56	166.06	0.56			DvH	2021RUS
		249.80	g		-1937.5	1.7	185.4	1.7			R	2019DIK
		249.80	g		-1937.48	0.88	185.40	0.88			E	1945WAG
		249.80	l	SEL	-1918.5	3.8	166.5	3.8	19.58	0.51	v	2019DIK
C_4H_6	1-butyne	281.18	g	SEL	-2598.06	0.67	166.68	0.67			TN	2021RUS
		281.18	l	SEL1	-2574.36	0.71	142.98	0.71			DvH	2021RUS
		281.18	g		-2596.61	1.06	165.23	1.06			R	2019DIK
		281.18	g		-2596.76	0.84	165.38	0.84			C	1951PRO
		281.18	g		-2597.5	2.1	166.1	2.1			E	1945WAG
		281.18	g		-2596.80	0.88	165.42	0.88			C	1945WAG
		281.18	l		-2572.60	1.09	141.22	1.09	24.00	0.23	R	2019DIK
		281.18	lg						23.79		R	1985MAJ
		281.18	lg	SEL					23.7		v	1971WIL
		281.18	lg						23.38			1950AST
	2-butyne	300.12	l	SEL	-2551.15	0.58	119.77	0.57			DvH	2021RUS
		300.12	g	SEL1	-2577.85	0.49	146.47	0.49			TN	2021RUS
		300.12	g		-2576.9	2.9	145.5	2.9			R	2019DIK
		300.12	g		-2576.7	1.0	145.3	1.0			C	1951PRO
		300.12	g		-2579.4	0.2	148.0	0.2			E	1945WAG
		300.12	l		-2550.3	2.9	118.9	2.9	26.62	0.48	R	2019DIK
		300.12	lg	SEL					26.7		v	1971WIL
C_5H_8	1-pentyne	313.51	l	SEL	-3226.6	2.3	115.9	2.3			DvH	1945WAG
		313.51	g	SEL1	-3255.0	2.1	144.3	2.1			E	1945WAG
		313.51	g		-3255.0	4.2	144.4	4.2			R	2019DIK

		313.51	l		-3228.9	4.3	118.3	4.3	26.09	1.09	R	2019DIK
		313.51	lg	SEL					28.4		v	1971WIL
	2-pentyne	329.27	l	SEL	-3208.8	2.2	98.1	2.2			DvH	1945WAG
		329.27	g	SEL1	-3239.6	2.1	128.9	2.1			E	1945WAG
		329.27	g		-3239.6	4.2	128.9	4.2			R	2019DIK
		329.27	l		-3213.4	4.3	102.8	4.3	26.12	1.14	R	2019DIK
		329.27	lg	SEL					30.8		v	1971WIL
C_6H_{10}	1-hexyne	344.53	l	SEL	-3879.3	1.6	89.4	1.6			DvH	1979ROG
		344.53	g	SEL1	-3912.3	1.2	122.3	1.2			H2	1979ROG
		344.53	g		-3914.3	2.1	124.3	2.1			R	2019DIK
		344.53	l	SEL	-3881.3	2.1	91.4	2.1	32.94	0.29	v	2019DIK
	2-hexyne	357.59	l	SEL	-3861.9	2.5	71.9	2.5			DvH	1979ROG
		357.59	g	SEL1	-3897.7	2.4	107.7	2.4			H2	1979ROG
		357.59	g		-3894.6	7.5	104.6	7.5			R	2012KRO
		357.59	l		-3859.0	7.6	69.0	7.6	35.6		R	2012KRO
		357.59	lg	SEL					35.8		v	2007BOU
	3-hexyne	354.58	l	SEL	-3860.2	1.9	70.2	1.9			DvH	1979ROG
		354.58	g	SEL1	-3895.4	1.9	105.4	1.9			H2	1979ROG
		354.58	g		-3900.1	2.6	110.1	2.6			R	2019DIK
		354.58	l	SEL	-3864.8	2.6	74.9	2.6	35.21	0.29	v	2019DIK
C_4H_4	butenyne	279.18	g	SEL	-2434.97	0.58	289.41	0.58			TN	2021RUS
		279.18	l	SEL1	-2411.8	2.1	266.2	2.1	23.21	0.40	TN	2021RUS
		279.18	g		-2434.4	2.8	288.9	2.8			R	2019DIK
		279.18	g		-2440.6	5.0	295.0	5.0			QM	1991ROT
		279.18	l		-2411.5	2.9	266.0	2.9	22.86	0.76	R	2019DIK
		279.18	l		-2380.0		234.4				C	1948REP
C_5H_6	3-penten-1-yne	317.05	l	SEL	-3050.7	3.6	225.9	3.6	27.58	1.50	R	2019DIK
		317.05	g	SEL1	-3078.3	3.3	253.4	3.3			R	2019DIK
	3-penten-1-yne, (E)-	323.65	l	SEL	-3050.7	3.2	225.9	3.2	28.35	1.54	R	2019DIK
		323.65	g	SEL1	-3079.1	2.8	254.2	2.8			R	2019DIK
		323.65	g		-3083.9	5.0	259.0	5.0			QM	1991ROT
	3-penten-1-yne, (Z)-	317.15	l	SEL	-3050.2	2.9	225.4	2.9	27.28	0.77	R	2019DIK
		317.15	g	SEL1	-3077.5	2.8	252.6	2.8			R	2019DIK
		317.15	g		-3082.9	5.0	258.0	5.0			QM	1991ROT
C_4H_2	butadiyne	283.65	g	SEL	-2319.73	0.58	460.00	0.58			TN	2021RUS
		283.65	l	SEL1	-2296.49	1.17	436.76	1.16			DvH	2021RUS
		283.65	g		-2320.4	2.9	460.7	2.9			R	2019DIK

		283.65	g		-2323.7		464.0				D	1992KIE
		283.65	l	SEL	-2297.1	3.1	437.4	3.1	23.24	1.01	v	2019DIK
Cycloalkanes												
C_3H_6	cyclopropane	240.27	g	SEL	-2091.75	0.40	53.84	0.40			TN	2021RUS
		240.27	l	SEL1	-2073.63	0.53	35.72	0.53	18.12	0.20	TN	2021RUS
		240.27	g		-2074.33	0.62	36.43	0.62			R	2019DIK
		240.27	g		-2077.2		39.3				HBr	1950LAC
		240.27	g		-2091.37	0.54	53.47	0.55			C	1949KNO
		240.27	l		-2091.2	0.5	53.3	0.5	16.88	0.37	R	2019DIK
		240.27	lg						18.11		R	1985MAJ
		240.27	lg						17.02			1970LIN
		240.27	lg						17.02			1970LIN
C_4H_8	cyclobutane	285.64	g	SEL	-2745.02	0.39	27.81	0.39			TN	2021RUS
		285.64	l	SEL1	-2721.14	0.40	3.93	0.40	23.88	0.30	TN	2021RUS
		285.64	g		-2743.9	1.4	26.7	1.4			R	2019DIK
		285.64	l		-2720.8	1.3	3.6	1.3	23.04	0.47	R	2019DIK
		285.64	l		-2720.4	0.5	3.2	0.5	23.20		C	1952KAA
		285.64	lg						23.92		R	1985MAJ
		285.64	lg						23.26	0.40		1950COO
C_5H_{10}	cyclopentane	322.40	l	SEL	-3291.40	0.43	-105.11	0.42	28.69	0.20	TN	2021RUS
		322.40	g	SEL1	-3320.09	0.43	-76.42	0.42			TN	2021RUS
		322.40	g		-3319.8	1.2	-76.7	1.2			R	2019DIK
		322.40	g		-3320.11	0.80	-76.40	0.79			R	1959MCC
		322.40	l		-3291.37	1.19	-105.14	1.19	28.41	0.34	R	2019DIK
		322.40	l		-3291.2	1.3	-105.3	1.3			C	1947SPI
		322.40	l		-3290.90	0.71	-105.61	0.71	28.66		C	1946PRO
		322.40	lg						28.72		R	1985MAJ
		322.40	lg						28.50			1971WIL
		322.40	lg						28.58	0.10		1959MCC
		322.40	lg						28.90			1952KAA
		322.40	lg						29.29			1947SPI
		322.40	lg						29.20			1943AST
	methylcyclobutane	310.00	l	SEL	-3339.5	1.3	-57.1	1.3			DvH	1950HUM
		310.00	g	SEL1	-3352.0	1.3	-44.5	1.3			C	1950HUM
		310.00	g		-3391.3	2.6	-5.2	2.6			R	2019DIK
		310.00	l	SEL	-3365.4	2.9	-31.1	2.9	25.92	1.30	v	2019DIK
C_6H_{12}	cyclohexane	353.87	l	SEL	-3919.73	0.30	-156.08	0.29	33.14	0.15	TN	2021RUS

	353.87	g	SEL1	-3952.87	0.31	-122.94	0.30			TN	2021RUS
	353.87	l		-3952.28	0.79	-123.53	0.78			R	2019DIK
	353.87	l		-3919.28	0.76	-156.53	0.76	33.00	0.21	R	2019DIK
	353.87	l		-3918.6	0.7	-157.2		33.50		C	1952KAA
	353.87	l		-3918.4	1.0	-157.4	1.0	33.47		C	1947SPI
	353.87	l		-3919.90	0.71	-155.91	0.71	33.1		C	1946PRO
	353.87	l		-3919.6	1.3	-156.2	1.3			C	1940MOO
	353.87	l		-3917.98	0.75	-157.83				C	1939MOO
	353.87	l		-3935.3		-140.5				C	1915RIC
	353.87	l		-3946.8		-129.0				C	1901ZUB
	353.87	lg						33.10			1995DIO
	353.87	lg						33.12		R	1985MAJ
	353.87	lg						32.79	0.14		1982JOC
	353.87	lg						33.00	0.10		1982FUR
	353.87	lg						33.00			1981SHI
	353.87	lg						33.00	0.10		1979MAJ
	353.87	lg						32.90	0.30		1972SAB
	353.87	lg						32.90	0.30		1972SAB
	353.87	lg						33.00			1971WIL
	353.87	lg						32.90			1971MOR
	353.87	lg						33.00	0.10		1960WAD
	353.87	lg						30.12			1957GLA
	353.87	lg						33.04			1956BRE
	353.87	lg						33.03			1947OSB
	353.87	lg						33.10			1946PRO2
	353.87	lg						33.30	0.10		1943AST
	353.87	lg						33.50			1927NAG
	353.87	lg						30.17	0.29		1926MAT
methylcyclopentane	344.96	l	SEL	-3937.74	0.37	-138.07	0.36	31.78	0.15	TN	2021RUS
	344.96	g	SEL1	-3969.52	0.38	-106.29	0.37			TN	2021RUS
	344.96	g		-3968.9	1.5	-106.9	1.5			R	2019DIK
	344.96	l		-3937.4	1.4	-138.5	1.4	31.59	0.22	R	2019DIK
	344.96	l		-3938.32	0.59	-137.50	0.59			C	1969GOO
	344.96	l		-3937.70	0.75	-138.11	0.75	31.7		C	1946PRO
	344.96	l		-3936.2	1.7	-139.6	1.7			C	1940MOO
	344.96	l		-3956.4		-119.4				C	1901ZUB
	344.96	lg						31.78		R	1985MAJ

		344.96	lg						31.60			1971WIL
		344.96	lg						31.71			1960SCO
		344.96	lg						31.63	0.10		1947OSB
C_7H_{14}	methylcyclohexane	374.12	l	SEL	-4565.29	0.96	-189.82	1.05	35.40	0.20	C	1946PRO
		374.12	g	SEL1	-4600.69	1.08	-154.42	1.08			DvH	1946PRO
		374.12	g		-4600.2	1.7	-154.9	1.7			R	2019DIK
		374.12	l		-4564.9	1.6	-190.2	1.6	35.33	0.27	R	2019DIK
		374.12	l		-4564.3	1.9	-190.8	1.9			C	1940MOO
		374.12	lg						35.10	0.40		1987AZA
		374.12	lg						35.44		R	1985MAJ
		374.12	lg						35.40	0.10		1979MAJ
		374.12	lg						35.40	0.29		1978FUC
		374.12	lg						35.30			1975KUS
		374.12	lg						35.23	0.17		1966WAD2
		374.12	lg						35.35			1947OSB
		374.12	lg						31.59	0.01		1926MAT
$C_{10}H_{20}$	1,3-diethylcyclohexane	445.70	l	SELu	-6515.9	6.2	-277.1	6.2	46.83	1.55	R	2019DIK
		445.70	g	SEL1u	-6562.7	6.0	-230.3	6.0			R	2019DIK
Cycloalkenes												
C_4H_6	cyclobutene	275.74	g	SEL	-2591.98	0.71	160.60	0.71			TN	2021RUS
		275.74	l	SEL1	-2569.73	0.74	138.35	0.74			DvH	2021RUS
		275.74	g		-2588.1	1.6	156.7	1.6			R	2019DIK
		275.74	g		-2588.2	1.5	156.8	1.5			C	1968WIB
		275.74	l	SEL	-2565.8	1.7	134.4	1.7	22.26	0.21	v	2019DIK
C_5H_8	cyclopentene	317.39	l	SEL	-3117.56	0.52	6.88	0.52	28.29	0.30	TN	2021RUS
		317.39	g	SEL1	-3145.85	0.47	35.17	0.47			TN	2021RUS
		317.39	g		-3142.63	0.99	31.94	0.99			R	2019DIK
		317.39	g		-3146.2		35.6				H2	1982ALL
		317.39	g		-3145.0		34.3				E	1970FUR
		317.39	l		-3114.77	0.93	4.09	0.93	27.86	0.34	R	2019DIK
		317.39	l		-3115.20	0.59	4.51	0.59	28.29		C	1961LAB
		317.39	l		-3115.54	0.67	4.85	0.67	28.35		E	1949EPS
		317.39	lg						28.37			1941LIS
	methylenecyclobutane	315.00	l	SEL	-3204.7	0.5	94.0	0.5	27.70	0.42	C	1974GOO
		315.00	g	SEL1	-3232.40	0.65	121.72	0.65			C	1974GOO
		315.00	g		-3230.8	1.6	120.1	1.6			R	2019DIK
		315.00	g		-3217.0	5.0	106.3	5.0			QM	1991ROT

		315.00	l		-3204.5	0.9	93.8	0.9	26.24	1.29	R	2019DIK
C_6H_{10}	cyclohexene	356.10	l	SEL	-3752.00	0.32	-37.99	0.31	33.56	0.53	TN	2021RUS
		356.10	g	SEL1	-3785.56	0.33	-4.43	0.32			TN	2021RUS
		356.10	g		-3785.32	1.07	-4.67	1.07			R	2019DIK
		356.10	l		-3751.90	1.03	-38.09	1.03	33.42	0.29	R	2019DIK
		356.10	l		-3752.39	0.49	-37.60	0.49	33.50	0.53	C	1996STE
		356.10	l		-3752.0	0.5	-38.0	0.5			C	1969GOO
		356.10	l		-3751.5	0.5	-38.5	0.5			C	1961LAB
		356.10	l		-3749.39	0.79	-40.60	0.79			E	1949EPS
		356.10	lg									1996STE
		356.10	lg						33.57		R	1985MAJ
		356.10	lg						30.50	0.25		1926MAT
Bicycloalkanes												
$C_{10}H_{12}$	tetralin	480.56	l	SEL	-5621.5	1.0	-28.2	1.0			C	1976GOO
		480.56	g	SEL1	-5676.5	1.4	26.8	1.4			DvH	1976GOO
		480.56	g		-5675.7	2.0	26.0	2.0				1971BOY
		480.56	l		-5598.6		-51.1				C	1953KAR
		480.56	l		-5581.9		-67.8				C	1951HOC
		480.56	lg	SEL					55.00	1.00	v	1971BOY
		480.56	lg						58.60			1971BOY
$C_{10}H_{18}$	cis-decalin	468.93	l	SEL	-6287.7	1.3	-219.5	1.3	50.2	2.1	C	1941DAV
		468.93	g	SEL1	-6337.9	2.5	-169.3	2.5			DvH	1941DAV
		468.93	g		-6338.2	1.9	-169.0	1.9			R	2019DIK
		468.93	g		-6338.0	2.3	-169.2	2.3			DvH	1960SPE
		468.93	l		-6287.7	1.6	-219.5	1.6	50.47	0.91	R	2019DIK
		468.93	l		-6288.2	0.9	-219.0	0.9			C	1960SPE
		468.93	l		-6275.6		-231.6				C	1926HUC
		468.93	l		-6280.9	4.1	-226.3				C	1925ROT
		468.93	lg	SEL					50.2	2.1	v	1960SPE
	trans-decalin	460.42	l	SEL	-6278.9	1.3	-228.3	1.3			C	1941DAV
		460.42	g	SEL1	-6327.4		-179.8				DvH	1941DAV
		460.42	g		-6325.2	2.8	-182.0	2.8			R	2019DIK
		460.42	g		-6325.0	2.3	-182.2	2.3			DvH	1960SPE
		460.42	l		-6277.0	2.6	-230.2	2.6	48.15	0.99	R	2019DIK
		460.42	l		-6276.96	0.92	-230.23	0.92			C	1960SPE
		460.42	l		-6263.9	2.1	-243.3				C	1937HUC
		460.42	l		-6255.9		-251.3				C	1926HUC

		460.42	l		-6268.2	4.6	-239.0				C	1925ROT
		460.42	lg	SEL					48.5	2.1	v	1960SPE
		460.42	lg						42.84			1957GLA
$C_{12}H_{22}$	1,1'-bicyclohexyl	511.10	l	SEL	-7593.0	1.2	-272.8	1.2			C	1976GOO
		511.10	g	SEL1	-7651.0	0.3	-214.8	1.2			DvH	1976GOO
		511.10	g		-7650.6	3.0	-215.2	3.0			R	2012KRO
		511.10	g		-7647.4	3.1	-218.4	3.1			DvH	1978MON
		511.10	l		-7592.0	2.3	-273.8	2.3	58.60	1.90	R	2012KRO
		511.10	l		-7589.9	2.6	-275.9	2.6	57.99	0.25	C	1978MON
		511.10	l		-7439.7		-426.1				C	1962GOL
		511.10	l		-7596.5		-269.3				C	1951WIS
		511.10	l		-7537.5	6.3	-328.3				C	1935BRU
		511.10	lg						58.90	1.70	R	2019DIK
		511.10	lg	SEL					57.98		v	1985MAJ
$C_{10}H_{12}$	tetralin	480.56	l	SEL	-5621.5	0.9	-28.2	1.0			C	1976GOO
		480.56	g	SEL1	-5676.54	1.05	26.82	1.04			DvH	1976GOO
		480.56	g		-5674.2	4.6	24.5	4.6			R	2019DIK
		480.56	l		-5620.6	4.0	-29.1	4.0	53.6	2.2	R	2019DIK
		480.56	l		-5617.5	2.1	-32.2	2.2			C	1971BOY
		480.56	lg	SEL					55.00	0.30	v	1971BOY
Aromatic Hydrocarbons												
C_6H_6	benzene	353.22	l	SEL	-3267.51	0.23	49.18	0.22	33.94	0.15	TN	2021RUS
		353.22	g	SEL1	-3301.45	0.23	83.12	0.22			TN	2021RUS
		278.70	s	SEL2	-3256.83	0.92	38.50	0.92	10.50	0.20	DfusH	2008ROU
		353.22	g		-3301.20	0.76	82.86	0.76			R	2019DIK
		353.22	g		-3301.2	0.9	82.9	0.9			R	2008ROU
		353.22	l		-3267.34	0.75	49.01	0.75	33.85	0.14	R	2019DIK
		353.22	l		-3267.49	0.42	49.16	0.42			C	1969GOO
		353.22	l		-3276.1		57.7				C	1948REP
		353.22	l		-3266.95	0.38	48.62				C	1947COO
		353.22	l		-3267.62	0.42	49.29	0.42	33.94		C	1945PRO
		353.22	l		-3264.8		46.4				C	1929LAN
		353.22	l		-3277.7		59.4				C	1925BAR
		353.22	l		-3271.3		52.9				C	1920RIC
		353.22	l		-3246.8		28.5				C	1918GUI
		353.22	l		-3267.2		48.9				C	1915RIC
		353.22	lg						33.92	0.06	R	2008ROU

		353.22	lg						33.90	0.10	R	2002MAN
		353.22	lg						33.74	0.11		1987SAB
		353.22	lg						33.80	0.10		1973SVO
		353.22	lg						33.90	0.10		1973KON
		353.22	lg						33.90			1971WIL
		353.22	lg						33.85			1957AND
		353.22	lg						33.84			1947OSB
		353.22	lg						34.00			1927NAG
		353.22	lg						30.84	0.13		1926MAT
		278.70	sl	SEL					10.50	0.20	f	2008ROU
C_7H_8	toluene	383.75	l	SEL	-3909.71	0.34	12.07	0.33	38.04	0.25	TN	2021RUS
		383.75	g	SEL1	-3947.7		50.1				TN	2021RUS
		178.20	s	SEL2	-3899.8	1.5	2.1	1.5	9.90	1.10	R	2008ROU
		383.75	g		-3947.75	0.92	50.11	0.92			R	2019DIK
		383.75	g		-3947.74	1.10	50.10	1.10			R	2008ROU
		383.75	l		-3909.66	0.89	12.02	0.89	38.09	0.25	R	2019DIK
		383.75	l		-3909.68	1.05	12.04	1.05			R	2008ROU
		383.75	l		-3909.9	0.5	12.3	0.5	38.04		C	1945PRO
		383.75	l		-3938.4		40.8				C	1925BAR
		383.75	l		-3913.0		15.4				C	1920RIC
		383.75	l		-3920.7		23.1				C	1915RIC
		383.75	l		-3927.0		29.4				C	1906SCH
		383.75	lg						38.06	0.04	R	2008ROU
		383.75	lg						38.10	0.10	R	2002MAN
		383.75	lg						37.79	0.13		1982JOC
		383.75	lg						38.00			1971WIL
		383.75	lg						38.14			1957AND
		383.75	lg						37.99			1947OSB
		383.75	lg						33.35	0.04		1926MAT
C_8H_{10}	ethylbenzene	408.96	l	SEL	-4564.41	0.55	-12.53	0.55	42.26	0.40	TN	2021RUS
		408.96	g	SEL1	-4606.67	0.55	29.73	0.55			TN	2021RUS
		408.96	g		-4605.8	3.3	28.8	3.3			R	2019DIK
		408.96	l		-4563.3	3.2	-13.7	3.2	42.49	0.43	R	2019DIK
		408.96	l		-4562.4	1.0	-14.5	1.0			C	1953COO
		408.96	l		-4564.87	0.71	-12.07	0.71	42.26		C	1945PRO
		408.96	l		-4566.4		-10.5				C	1922AUW
		408.96	l		-4557.6		-19.3				C	1922AUW

	408.96	l		-4565.9		-11.0				C	1915RIC
	408.96	lg						42.40	0.10		1981HOS
	408.96	lg						42.30			1971WIL
	408.96	lg						42.24	0.10		1947OSB
	408.96	lg						36.02	0.17		1926MAT
m-xylene	412.25	l	SEL	-4551.86	0.63	-25.08	0.63	42.60	0.30	C	1946PRO
	412.25	g	SEL1	-4594.46	0.69	17.52	0.69			DvH	1946PRO
	412.25	lg		-4551.6	1.3	-25.4	1.3	42.77	0.28	v	2019DIK
	412.25	g		-4594.3	1.4	17.4	1.4			R	2019DIK
	412.25	l		-4549.56	0.54	-27.38	0.54			C	1946COO
	412.25	l		-4567.6		-9.3				C	1915RIC
	412.25	l		-4581.4		4.5				C	1910RIC
	412.25	lg						42.70			1971WIL
	412.25	lg						36.36			1957GLA
	412.25	lg						43.04			1957AND
	412.25	lg						42.65	0.10		1947OSB
	412.25	lg						42.60			1946PRO
	412.25	lg						36.36	0.38		1926MAT
o-xylene	417.56	l	SEL	-4552.9	1.0	-24.1	1.0	43.40	0.30	C	1945PRO
	417.56	g	SEL1	-4596.26	1.04	19.32	1.04			DvH	1945PRO
	417.56	g		-4595.9	1.8	19.0	1.8			R	2019DIK
	417.56	l		-4552.4	1.8	-24.5	1.8	43.48	0.26	R	2019DIK
	417.56	l		-4551.5	0.5	-25.5	0.5			C	1946COO
	417.56	l		-4567.6		-9.3				C	1915RIC
	417.56	l		-4581.4		4.5				C	1910RIC
	417.56	lg						42.90			1995CHI
	417.56	lg						43.40			1971WIL
	417.56	lg						36.90			1957GLA
	417.56	lg						43.96			1957AND
	417.56	lg						43.43	0.10		1947OSB
	417.56	lg						43.40			1945PRO2
	417.56	lg						36.82	0.38		1926MAT
p-xylene	411.47	l	SEL	-4552.86	0.92	-24.08	0.92	42.30	0.30	C	1946PRO
	411.47	g	SEL1	-4595.16	0.97	18.22	0.97			C(l)	1946PRO
	411.47	g		-4594.6	2.2	17.7	2.2			R	2019DIK
	411.47	l		-4552.4	1.9	-24.5	1.9	42.20	1.08	R	2019DIK
	411.47	l		-4551.4	0.5	-25.5	0.5			C	1946COO

		411.47	l		-2254.7		-25.2				C	1915RIC
		411.47	l		-4565.9		-11.0				C	1910RIC
		411.47	lg						42.30			1995CHI
		411.47	lg						43.00	0.10		1990SMI
		411.47	lg						42.35	0.10		1988MES
		411.47	lg						42.30	0.10		1981HOS
		411.47	lg						42.60			1974AMB
		411.47	lg						42.40			1971WIL
		411.47	lg						35.94			1957GLA
		411.47	lg						42.72			1957AND
		411.47	lg						42.37	0.10		1947OSB
		411.47	lg						42.30			1946PRO
		411.47	lg						35.98	0.08		1926MAT
C_9H_{12}	isopropylbenzene	425.54	l	SEL	-5215.44	0.96	-40.80	0.97			C	1945PRO
		425.54	g	SEL1	-5260.54	1.09	4.30	1.09			DvH	1945PRO
		425.54	g		-5260.2	1.7	4.0	1.7			R	2019DIK
		425.54	l		-5215.1	1.6	-41.1	1.6	45.10	0.39	DvH	2019DIK
		425.54	l		-5218.6		-37.6				C	1915RIC
		425.54	lg						45.10			1994RUI
		425.54	lg						45.10	0.10		1982FUC
		425.54	lg						44.00			1975KUS
		425.54	lg						45.10			1971WIL
		425.54	lg						37.03			1957GLA
		425.54	lg	SEL					45.14		v	1947OSB
		425.54	lg						45.10			1945PRO2
$C_{10}H_{14}$	m-isopropyltoluene	448.35	l	SEL	-5857.3	1.0	-78.2	1.0			C	1973GOO
		448.35	g	SEL1	-5906.9	1.3	-28.7	1.3			DvH	1973GOO
		448.35	g		-5905.9	1.9	-29.7	1.9			R	2019DIK
		448.35	l	SEL	-5856.3	1.7	-79.2	1.7	49.55	0.88	v	2019DIK
		448.35	l		-5857.8	2.2	-77.7	2.2			C	1946PRO
		448.35	lg						50.00			1971WIL
	o-isopropyltoluene	451.50	l	SEL	-5862.62	0.84	-72.92	0.84			C	1973GOO
		451.50	g	SEL1	-5912.26	1.19	-23.28	1.19			DvH	1973GOO
		451.50	g		-5911.3	1.8	-24.2	1.8			R	2019DIK
		451.50	l	SEL	-5861.7	1.6	-73.9	1.6	49.64	0.84	v	2019DIK
		451.50	l		-5859.9	2.2	-75.6	2.2			C	1946PRO
		451.50	lg						50.60			1971WIL

	p-isopropyltoluene	450.27	l	SEL	-5857.9	1.0	-77.6	1.0			C	1973GOO
		450.27	g	SEL1	-5907.28	1.11	-28.26	1.10			DvH	1973GOO
		450.27	g		-5906.3	1.7	-29.3	1.7			R	2019DIK
		450.27	l	SEL	-5856.9	1.6	-78.7	1.6	49.39	0.47	v	2019DIK
		450.27	l		-5857.6	2.2	-77.9	2.2			C	1946PRO
		450.27	lg						49.20			2005HOS
		450.27	lg						48.90			1994RUI
		450.27	lg						50.30			1971WIL
C_8H_8	styrene	418.45	l	SEL	-4395.42	0.48	104.31	0.48	44.03	0.40	TN	2021RUS
		418.45	g	SEL1	-4439.45	0.48	148.34	0.48			TN	2021RUS
		418.45	g		-4439.1	1.5	148.0	1.5			R	2019DIK
		418.45	l		-4394.9	1.4	103.8	1.4	44.16	0.60	R	2019DIK
		418.45	l		-4395.63	0.59	104.52	0.59	43.93	0.42	C	1947ROB
		418.45	l		-4394.87	0.84	103.76	0.84	43.50		C	1945PRO
		418.45	l		-4399.5		108.4				C	1929LAN
		418.45	lg						43.93	0.42		1946PIT
		418.45	lg						43.20			1939PAT
$C_{10}H_8$	naphthalene	353.65	s	SEL	-5154.7	3.4	78.0	1.5	16.90	0.70	R	2008ROU
		353.65	l	SEL1	-5173.0	1.7	94.9	1.7			DvH	2008ROU
		491.11	g	SEL2	-5228.7	1.5	150.6	1.5			R	2008ROU
		491.11	g		-5228.4	1.5	150.3	1.5			R	2019DIK
		491.11	g		-5229.7	1.9	151.7	1.9			DfusH	1960SPE
		353.65	l		-5173.3	2.1	95.2	2.1	55.40	1.40	DvH	2008ROU
		491.11	lg						54.64	0.95		2008ZHA
		491.11	lg	SEL					55.40	1.40	v	2008ROU
		491.11	lg						60.30	1.10		2006HAF
		491.11	lg						53.40			1998CHI
		491.11	lg						56.60			1995CHI
		491.11	lg						54.80	0.40		1993CHI
		491.11	lg						55.00	1.20		1981DEK
		491.11	lg						55.10	1.10		1968FOW
		491.11	lg						56.4	2.0		1955CAM
		491.11	lg						55.50	1.80		1923MOR
		353.65	s		-5155.9	0.1	77.8	1.5			R	2019DIK
		353.65	s		-5150.1		72.0				C	1996BAL
		353.65	s		-5153.9	5.1	75.8	5.1			C	1983HOL
		353.65	s		-5156.4	0.6	78.3	0.6			C	1977AMM

		353.65	s		-5156.15	0.92	78.09	0.92			C	1966COL
		353.65	s		-5156.9	1.6	78.8	1.6			C	1960SPE
		353.65	s		-5156.8		78.8				C	1932MIL
		353.65	s		-5151.2	0.2	73.1	0.2			C	1931KEF
		353.65	s		-5152.7		74.7				C	1931BUR
		353.65	sg						72.47	0.06		2019DIK
		353.65	sg						72.60	0.30		2008ROU
		353.65	sg						70.4			1998CHI
		353.65	sg						72.30	0.40		1988TOR
		353.65	sg						72.60	0.10		1983EKE
		353.65	sg						72.40	0.70		1982MUR
		353.65	sg						72.5			1974SIN
		353.65	sg						72.10	0.25		1972MOR
		353.65	sg						73.00	0.25		1972IRV
		353.65	sg						72.9			1966COL
		353.65	sg						72.70	0.30		1963MIL
		353.65	sg						73.2	3.1		1960SPE
		353.65	sl	SEL					16.90	0.70	f	2008ROU
		353.65	sl						16.80	0.40		2002CHI
		353.65	sl						16.81	0.70		2001RIJ
		353.65	sl						16.80	0.70		1993CHI
		353.65	sl						16.73	0.70		1981DEK
		353.65	sl						16.90	0.70		1980AND
		353.65	sl						16.80	0.70		1957MCC
$C_{11}H_{10}$	1-methylnaphthalene	517.84	l	SEL	-5814.0	1.7	56.7	1.7	60.10	0.80	C	1960SPE
		517.84	g	SEL1	-5874.1	1.9	116.8	1.9			DvH	1960SPE
		242.52	s	SEL2	-5807.1	1.7	49.7	1.7			DfusH	1960SPE
		517.84	g		-5873.0	2.7	115.6	2.7			R	2019DIK
		517.84	gl						65.10	1.10		2006HAF
		517.84	l		-5813.6	2.3	56.3	2.3	59.32	1.44	R	2019DIK
		517.84	l		-5783.0	5.8	25.6				C	1996BAL
		517.84	l		-5627.5		-129.9				C	1954HIP
		517.84	lg						65.10	1.10		2006HAF
		517.84	lg	SEL					60.10	0.80	v	2003VER
		517.84	lg						62.4			2002LEI
		517.84	lg						57.32	0.42		1974SAB
		517.84	lg						60.7	2.1		1960SPE

		517.84	lg						46.48			1957GLA
		242.52	sl	SEL					6.95	1.00	f	1996DOM
	2-methylnaphthalene	307.69	s	SEL	-5802.7	1.5	45.3	1.5	12.13	1.00	C	1960SPE
		514.25	l	SEL1	-5814.8	2.2	57.5	2.4			DfusH	1960SPE
		514.25	g	SEL2	-5860.1	1.8	102.8	2.6			DvH	1960SPE
		514.25	g	u	-5867	12	110	12			R	2019DIK
		514.25	l	u	-5815	8	58	8	58.69		R	2019DIK
		307.69	s	u	-5796	11	39	11	70.6	5.0	R	2019DIK
		514.25	lg	SEL					45.31	1.00	v	1957GLA
		307.69	s		-5792.7	2.2	35.3	2.2			C	1939RIC
		307.69	sl	SEL					12.13	1.00	f	1996DOM
C_8H_8	styrene	418.45	l	SEL	-4394.87	0.84	103.76	0.84	43.50	0.40	C	1945PRO
		418.45	g	SEL1	-4438.35	0.92	147.24	0.92			C	1945PRO
		418.45	l		-4395.63	0.59	104.52	0.59			C	1947ROB
		418.45	l		-4379.8	6.3	88.7	6.3			C	1938LUS
		418.45	l		-4374.4		83.3				C	1918GUI
		418.45	l		-4379.0		87.9				C	1914MOU
		418.45	l		-4431.3		140.2				C	1911LEM
		418.45	l		-4336.7		45.6				C	1910AUW
		418.45	lg						43.50	0.40		1946PIT
		418.45	lg						43.93	0.42		1946PIT
		418.45	lg						43.20			1939PAT

OXIDIZED HYDROCARBONS												
Carbon Oxides												
CO_2	carbon dioxide	194.69	g	SEL	0.000	0.021	-393.476	0.015			TN	2021RUS
		194.69	g		0.03	0.13	-393.51	0.13			R	2019DIK
		194.69	g		0.03	0.13	-393.51	0.13			R	1984COX
CO	carbon monoxide	81.64	g	SEL	-282.952	0.030	-110.524	0.026			TN	2021RUS
		81.64	g		-282.93	0.28	-110.55	0.28			R	2019DIK
		81.64	g		-282.95	0.17	-110.53	0.17			R	1984COX
		81.64	g		-283.036	0.146	-110.440	0.146			C	1933FEN
Alkanols												
CH_4O	methanol	337.63	l	SEL	-726.52	0.16	-238.61	0.15	37.70	0.05	TN	2021RUS
		337.63	g	SEL1	-764.22	0.16	-200.91	0.15			TN	2021RUS
		337.63	g		-763.44	0.92	-201.69	0.92			R	2019DIK
		337.63	g		-764.3		-200.8				E	1976HIN

		337.63	g		-763.68	0.20	-201.45				C	1932ROS
		337.63	l		-725.89	0.88	-239.24	0.88	37.55	0.27	R	2019DIK
		337.63	l		-726.8		-238.4				C	1972BAR
		337.63	l		-725.71	0.13	-239.41	0.13			C	1965CHA
		337.63	l		-726.51	0.21	-238.62	0.21			C	1960GRE
		337.63	l		-726.34	0.20	-238.79				C	1931ROS
		337.63	l		-715.0		-250.1				C	1925PAR
		337.63	l		-713.8		-251.3				C	1920RIC
		337.63	lg						37.80			2010SCH
		337.63	lg						38.00			2004NAS
		337.63	lg						37.83		R	1985MAJ
		337.63	lg						37.40	0.10		1973SVO
		337.63	lg						37.43	0.02		1971POL
		337.63	lg						37.30	0.10		1966WAD
		337.63	lg						37.70	0.10		1963MCC
		337.63	lg						37.40	0.04		1960GRE
		337.63	lg						35.30	0.04		1926MAT
C_2H_6O	ethanol	351.57	l	SEL	-1366.92	0.23	-277.51	0.22	42.47		TN	2021RUS
		351.57	g	SEL1	-1409.39	0.23	-235.04	0.22			TN	2021RUS
		351.57	g		-1409.8	1.2	-234.6	1.2			R	2019DIK
		351.57	l		-1367.24	1.12	-277.19	1.12	42.57	0.66	R	2019DIK
		351.57	l		-1367.58	0.25	-276.85	0.25			C	1965CHA
		351.57	l		-1366.95	0.42	-277.48	0.42	42.34	0.08	C	1960GRE
		351.57	l		-1366.31	0.40	-278.12	0.40			C	1932ROS
		351.57	l		-1366.9		-277.6					1929KEL
		351.57	l		-1370.9		-273.5				C	1925PAR
		351.57	l		-1368.3		-276.1				C	1920RIC
		351.57	l		-1368.6		-275.8				C	1911EME
		351.57	lg						42.30			2010SCH
		351.57	lg						41.70			2004NAS
		351.57	lg						42.40			1995DIO
		351.57	lg						42.26	0.02		1971POL
		351.57	lg						42.30	0.08		1966WAD
		351.57	lg						42.20	0.10		1963MCC
		351.57	lg						42.59			1961GRE
		351.57	lg						38.91	0.01		1926MAT
C_3H_8O	1-propanol	370.26	l	SEL	-2021.03	0.25	-302.70	0.24	47.46		TN	2021RUS

		370.26	g	SEL1	-2068.49	0.26	-255.24	0.25			TN	2021RUS
		370.26	g		-2068.2	2.3	-255.6	2.3			R	2019DIK
		370.26	l		-2020.1	2.2	-303.6	2.2	48.04	0.69	R	2019DIK
		370.26	l		-2021.31	0.25	-302.42	0.26			C	1975MOS
		370.26	l		-2020.7	1.3	-303.0	1.3	47.41	0.08	Hde	1972CON
		370.26	l		-2021.17	0.25	-302.56	0.25			C	1970DEK
		370.26	l		-2020.41	0.63	-303.32	0.63			C	1967BUC
		370.26	l		-2019.37	0.29	-304.37	0.30			C	1965CHA
		370.26	l		-2021.37	0.75	-302.36	0.76	47.86	0.21	C	1961SNE
		370.26	l		-2017.7	1.0	-306.1	1.0	47.50		C	1960GRE
		370.26	l		-2032.6		-291.1				C	1920RIC
		370.26	lg						46.30			2010SCH
		370.26	lg						45.70			2004NAS
		370.26	lg						47.80			2004LUB
		370.26	lg						49.20			1995CHI
		370.26	lg						47.49	0.02		1971POL
		370.26	lg						47.32	0.08		1966WAD
		370.26	lg						46.60			1963MCC
	isopropanol	355.39	l	SEL	-2004.83	0.36	-318.90	0.36	45.44	0.10	TN	2021RUS
		355.39	g	SEL1	-2050.27	0.36	-273.46	0.36			TN	2021RUS
		355.39	g		-2051.9	1.8	-271.8	1.8			R	2019DIK
		355.39	g		-2051.0		-272.8				E	1965BUC
		355.39	l		-2006.3	1.7	-317.5	1.7	45.65	0.62	R	2019DIK
		355.39	l		-2006.90	0.21	-316.83	0.22	45.73		C	1965CHA
		355.39	l		-2005.77	0.42	-317.96	0.42	45.90	0.21	C	1961SNE
		355.39	l		-2005.1		-318.6		44.40		C	1950PAR
		355.39	lg						44.00			2004NAS
		355.39	lg						45.34	0.02		1971POL
		355.39	lg						45.23	0.13		1966WAD
		355.39	lg						44.00			1963MCC
		355.39	lg						45.51			1963HAL
		355.39	lg						40.04	0.04		1926MAT
$C_4H_{10}O$	1-butanol	390.77	l	SEL	-2676.18	0.24	-326.85	0.25			C	1975MOS
		390.77	g	SEL1	-2728.68	0.39	-274.35	0.38			DvH	1975MOS
		390.77	g		-2726.9	2.8	-276.1	2.8			R	2019DIK
		390.77	g		-2723.04	0.92	-279.99	0.92			C	1960GRE
		390.77	l		-2674.4	2.6	-328.7	2.6	52.57	1.07	R	2019DIK

	390.77	l		-2636	115	-367				C	1973DEL
	390.77	l		-2676.01	0.24	-327.02	0.25			C	1969MOS
	390.77	l		-2675.61	0.45	-327.42	0.45	52.30		C	1969GUN
	390.77	l		-2677.43	0.63	-325.61	0.63			C	1965CHA
	390.77	l		-2670.44	0.42	-332.60	0.42			C	1960TJE
	390.77	l		-2674.87	0.84	-328.16	0.84	51.88	0.42	C	1960SKI
	390.77	l		-2670.4		-332.6				C	1928VER
	390.77	l		-2676.0		-327.0				C	1925PAR
	390.77	l		-2670.8		-332.3				C	1920RIC
	390.77	lg						51.70			2010SCH
	390.77	lg						48.40			2004NAS
	390.77	lg	SEL					52.50		v	1995CHI
	390.77	lg						55.20			1992GRA
	390.77	lg						52.10			1984LAW
	390.77	lg						52.34	0.02		1971POL
	390.77	lg						52.30	0.08		1966WAD
	390.77	lg						51.00	0.10		1963MCC
	390.77	lg						52.80	0.84		1960GRE
	390.77	lg						43.81	0.04		1926MAT
isobutanol	380.90	l	SEL	-2669.64	0.59	-333.39	0.59			C	1965CHA
	380.90	g	SEL1	-2720.48	0.59	-282.56	0.59			DvH	1965CHA
	380.90	g		-2720.5	1.2	-282.5	1.2			R	2019DIK
	380.90	l		-2669.18	1.13	-333.85	1.13	51.32	0.49	R	2019DIK
	380.90	l		-2668.4	0.9	-334.6	0.9	50.80		Hde	1975CON
	380.90	l		-2668.51	0.84	-334.52	0.84	50.70		C	1960SKI
	380.90	l		-2665.8		-337.2				C	1920RIC
	380.90	lg						48.80			1999ORT
	380.90	lg						50.76	0.03		1984MAJ
	380.90	lg						50.79	0.02		1971POL
	380.90	lg	SEL					50.84	0.08	v	1966WAD
	380.90	lg						49.80			1963MCC
	380.90	lg						42.89	0.01		1926MAT
tert-butanol	355.50	l	SEL	-2643.95	0.79	-359.08	0.80	46.30		C	1960SKI
	355.50	g	SEL1	-2689.7	1.5	-313.4	1.5			DvH	1960SKI
	298.87	s	SEL2	-2636.7	5.1	-366.4	5.1	7.24		R	2019DIK
	355.50	g		-2690.72	1.08	-312.31	1.08			R	2019DIK
	355.50	l		-2643.91	0.97	-359.13	0.96	46.81	0.49	R	2019DIK

		355.50	l		-2643.80	0.84	-359.24	0.84	46.60		H2O	1991WIB
		355.50	l		-2647.4		-355.6		45.94			1955TAF
		355.50	lg						47.40			2007MAL
		355.50	lg						45.40			1995CHI
		355.50	lg						46.94	0.02		1971POL
		355.50	lg						46.61	0.08		1966WAD
		355.50	lg						44.90			1963MCC
$C_5H_{12}O$	1-pentanol	410.90	l	SEL	-3330.91	0.28	-351.43	0.29			C	1975MOS
		410.90	g	SEL1	-3387.60	0.35	-294.74	0.34			DvH	1975MOS
		410.90	g		-3387.0	1.8	-295.4	1.8			R	2019DIK
		410.90	g		-3381.7	2.0	-300.6	2.0			C	1960GRE
		410.90	l		-3330.3	1.3	-352.1	1.3	56.69	1.21	R	2019DIK
		410.90	l		-3329.92	0.67	-352.42	0.67	-1615.00		C	1971HAY
		410.90	l		-3329.96	0.64	-352.38	0.64	56.94	0.17	C	1969GUN
		410.90	l		-3324.65	0.38	-357.69	0.38			C	1965CHA
		410.90	lg						55.40			2010SCH
		410.90	lg						55.40			2006NAS
		410.90	lg						57.40			1995CHI
		410.90	lg						57.80			1995CHI
		410.90	lg						56.94	0.17		1966WAD
		410.90	lg	SEL					56.69		v	1965CHA
		410.90	lg						57.74	1.05		1960GRE
	2-methyl-1-butanol	402.14	l	SEL	-3325.95	0.54	-356.39	0.55	54.56	1.26	C	1965CHA
		402.14	g		-3381.2	1.3	-301.2	1.3			R	2019DIK
		402.14	l		-3325.75	0.97	-356.59	0.96	55.41	0.79	R	2019DIK
		402.14	lg						54.10			1963MCC
	isopentanol	404.73	l	SEL	-3326.2	0.5	-356.1	0.5	55.02	1.26	C	1965CHA
		404.73	g	SEL1	-3381.2	1.4	-301.1	1.4			DvH	1965CHA
		404.73	g		-3381.9	1.2	-300.5	1.2			R	2019DIK
		404.73	g		-3326.6	1.6	-300.4	1.6			C	1987MAR
		404.73	l		-3326.00	0.94	-356.33	0.94	55.88	0.75	R	2019DIK
		404.73	l		-3326.6	1.6	-355.7	1.6			C	1987MAR
		404.73	lg						55.30			1995CHI
		404.73	lg						54.30			1963MCC
		404.73	lg						44.18	0.01		1926MAT
Sugars												
$C_2H_6O_2$	1,2-ethanediol	470.73	l	SEL	-1189.19	0.37	-455.24	0.37	65.87	0.20	TN	2021RUS

		470.73	g	SEL1	-1255.06	0.40	-389.37	0.40			TN	2021RUS
		470.73	g		-1256.6	5.0	-387.8	5.0			R	2019DIK
		470.73	g		-1250.0	2.8	-394.4	2.8				1990KNA
		470.73	l		-1189.9	2.1	-454.6	2.1	66.8	4.6	R	2019DIK
		470.73	l		-1184.6	2.8	-459.8	2.8			C	1990KNA
		470.73	l		-1188.84	0.67	-455.59	0.67	67.60		C	1972GAR
		470.73	l		-1190.2		-454.2				C	1952PAR
		470.73	l		-1188.67	0.84	-455.76	0.84	65.46		C	1947MCC
		470.73	l		-1189.59	0.71	-454.84	0.71	65.54		C	1946PAR
		470.73	l		-1202.61	1.21	-441.82	1.21			C	1942JUN
		470.73	l		-1191.4	1.2	-453.0	1.2			C	1937MOU
		470.73	lg						65.40	0.30		2005VAS
		470.73	lg						66.00	0.20		2004VER
		470.73	lg						66.20			2003DER
		470.73	lg						63.40	0.10		1999MOK
		470.73	lg						65.60	0.30		1988KNA
		470.73	lg						68.20	0.80		1981JOO
		470.73	lg						66.10	0.30		1981HAL
		470.73	lg						63.70	0.10		1981AMB
		470.73	lg									1972GAR
		470.73	lg						63.80			1937GAL
$C_3H_8O_2$	2-methoxyethanol	397.54	l	SEL	-1901.7	7.6	-422.0	7.6	45.1	2.7	H2O	1977GUT
		397.54	g	SEL1	-1947	8	-377	8			DvH	1977GUT
		397.54	g		-1950.9	2.7	-372.9	2.7			R	2019DIK
		397.54	l		-1905.1	2.8	-418.6	2.8	45.72	0.70	R	2019DIK
		397.54	l		-1882.8		-440.9		45.03		C	1947SIM
		397.54	lg						45.20	0.20		1971KUS2
$C_3H_8O_3$	glycerin	563.00	l	SEL	-1654.3	0.4	-669.4	0.4	91.70	0.90	C	1988BAS
		563.00	g	SEL1	-1746.00	0.99	-577.73	0.98			DvH	1988BAS
		563.00	s	SEL2	-1636.02	0.99	-687.71	0.98			DfusH	1988BAS
		563.00	g		-1743.9	3.2	-579.9	3.2			R	2019DIK
		563.00	l		-1654.5	1.2	-669.3	1.2	89.4	2.9	R	2019DIK
		563.00	l		-1654.1		-669.6				C	1952PAR
		563.00	l		-1655.3	1.0	-668.4	1.0	91.52		C	1946PAR
		563.00	l		-1665.1		-658.6				C	1911EME
		563.00	lg	SEL					85.77		v	1962ROS
		291.05	sl	SEL					18.28		f	1991ACR

$C_6H_{12}O_6$	alpha-D-glucose	415.0	s	SEL	-2805.0	1.3	-1270.8	1.3			C	1960PON
		706	g	SEL1	-2944	49	-1132	49			DsubH	1960PON
		706	g		-2940	49	-1136	49			R	2019DIK
		415.0	s		-2801.51	1.10	-1274.30	1.10			R	2019DIK
		415.0	sg	SEL					139	49	s	2019DIK
$C_6H_{10}O_5$	cellulose	553	s(d)		-2825.5	0.8	-964.5	0.8			C	1950JES
$C_6H_{12}O_6$	fructose	415.0	s(d)	SEL	-2810.4	0.3	-1265.4	0.3			C	1939CLA
$C_{12}H_{22}O_{11}$	sucrose	415.0	s(d)	SEL	-5643.4	1.8	-2222.4	1.8			C	1960PON
		415.0	s(d)		-5644.2		-2221.6				C	1939CLA
		415.0	s(d)		-5637.4	1.7	-2228.4	1.7			C	1935HUF
Ethers												
C_2H_6O	dimethyl ether	248.37	g	SEL	-1460.41	0.40	-184.02	0.40			TN	2021RUS
		248.37	l	SEL1	-1441.9	1.1	-202.5	1.1			DvH	2021RUS
		248.37	l	u	-1443.6	7.2	-200.8	7.2	18.60	0.97	R	2019DIK
		248.37	g		-1460.4	1.0	-184.0	1.0			R	2019DIK
		248.37	g		-1460.38	0.46	-184.05	0.46			C	1964PIL
		248.37	l		-1460.38	0.61	-202.55	0.61			DvH	1964PIL
		248.37	lg	SEL					18.50		v	1976AMB
C_3H_8O	ethyl methyl ether	280.59	g	SEL	-2106.41	0.58	-217.32	0.58			DvH	2021RUS
		280.59	l	SEL1	-2082.5	1.2	-241.2	1.2			TN	2021RUS
		280.59	g		-2107.32	1.36	-216.41	1.36			R	2019DIK
		280.59	g		-2107.40	0.63	-216.33	0.63			C	1964PIL
		280.59	l	SEL	-2083.4	1.9	-240.3	1.9	23.90	1.10	v	2019DIK
$C_4H_{10}O$	diethyl ether	307.56	l	SEL	-2725.25	0.82	-277.78	0.82	27.37	0.25	TN	2021RUS
		307.56	g	SEL1	-2752.62	0.82	-250.41	0.82			TN	2021RUS
		307.56	g		-2751.8	2.7	-251.2	2.7			R	2019DIK
		307.56	g		-2726.3	1.8	-276.7	1.8			C	1968PIH
		307.56	g		-2751.06	0.75	-251.97	0.76			C	1963PIL
		307.56	l		-2724.9	2.7	-278.2	2.7	26.95	0.22	R	2019DIK
		307.56	l		-2732.1	1.9	-270.9	1.9			C	1957MUR
		307.56	lg						27.14	0.10		1980MAJ
		307.56	lg						27.20			1976AMB
		307.56	lg						26.61			1968PIH
		307.56	lg						27.15	0.25		1926MAT
$C_6H_{14}O$	diisopropyl ether	341.49	l	SEL	-4010.4	1.3	-351.2	1.3			C	1965COL
		341.49	g	SEL1	-4043.1	1.4	-318.5	1.4			DvH	1965COL
		341.49	g		-4041.7	4.2	-319.9	4.2			R	2019DIK

		341.49	l		-4010.2	1.7	-351.5	1.7	32.11	0.21	R	2019DIK
		341.49	lg	SEL					32.70	0.50	v	2007EFI
		341.49	lg						32.26		R	1985MAJ
		341.49	lg						32.10	0.10		1980MAJ
Aldehydes												
CH_2O	formaldehyde	254.13	g	SEL	-570.088	0.096	-109.214	0.096			TN	2021RUS
		254.13	l	SEL1	-549.65	0.55	-129.65	0.55	20.44	0.54	TN	2021RUS
		254.13	g		-570.61	0.41	-108.70	0.41			R	2019DIK
		254.13	g		-570.78	0.42	-108.52	0.42			C	1970FLE
		254.13	g		-561.1		-118.2				C	1925WAR
		254.13	l		-550.17	0.68	-129.14	0.68	20.44	0.54	R	2019DIK
C_2H_4O	acetaldehyde	293.56	g	SEL	-1193.06	0.25	-165.54	0.25			TN	2021RUS
		293.56	l	SEL1	-1166.84	0.47	-191.76	0.47	26.22	0.40	TN	2021RUS
		293.56	g		-1192.4	2.6	-166.2	2.6			R	2019DIK
		293.56	g		-1187.9	1.5	-170.7	1.5			LiB	1991WIB
		293.56	l		-1167.5	2.6	-191.1	2.6	24.86	0.38	R	2019DIK
		293.56	lg						25.70			1991WIB
		293.56	lg						26.12		R	1985MAJ
		293.56	lg						26.90			1963BUL
C_3H_6O	propanal	321.19	l	SEL	-1821.20	0.36	-216.71	0.35	29.94	0.25	TN	2021RUS
		321.19	g	SEL1	-1851.14	0.26	-186.77	0.25			TN	2021RUS
		321.19	g	u	-1846	8	-192	8			R	2019DIK
		321.19	l	u	-1816	8	-221	8	29.63	0.34	R	2019DIK
		321.19	l		-1819.58	0.63	-218.32	0.63			LiB	1991WIB
		321.19	l		-1822.2	1.5	-215.7	1.5			Hde	1972CON
		321.19	l		-1817.66	0.96	-220.25	0.96			Hde	1967BUC
		321.19	l		-1816.53	0.75	-221.38	0.75			C	1962TJE
		321.19	lg						29.60			1991WIB
		321.19	lg						29.64	0.07	Hde	1972CON
		321.19	lg						29.66	0.42	Hde	1967BUC
		321.19	lg						29.50			1962TJE
C_4H_8O	butanal	347.95	l	SEL	-2477.72	0.84	-239.49	0.84	33.68	0.42	TN	2021RUS
		347.95	g	SEL1	-2511.40	0.85	-205.81	0.85			TN	2021RUS
		347.95	g		-2511.8	1.9	-205.4	1.9			R	2019DIK
		347.95	l		-2478.1	1.9	-239.1	1.9	33.68	0.30	R	2019DIK
		347.95	l		-2471.77	0.84	-245.43	0.84			LiB	1991WIB
		347.95	l		-2479.1	1.5	-238.1	1.5			Hde	1967BUC

		347.95	l		-2478.69	0.71	-238.52	0.71			C	1960TJE
		347.95	l		-2477.1	1.4	-240.1	1.4			C	1960NIC
		347.95	lg						33.20			1995CHI
		347.95	lg						33.60			1991WIB
		347.95	lg						33.68	0.42	Hde	1967BUC
C_3H_4O	1-propenal	264.25	g	SEL	-1687.9		-64.2	1.1			TN	2021RUS
		264.25	g	u	-1647		-105				R	1998LIA
		264.25	g	u	-1659		-93				ion	1997AUB
		264.25	g	u	-1655		-97				ion	1996BOU
		264.25	g		-1689.1		-63.0	2.6			R	2019DIK
	2-propenal	325.40	l	SEL	-1656.4	1.4	-95.7	1.4	30.00	0.30	TN	2021RUS
		325.40	g	SEL1	-1686.4	1.2	-65.7	1.2			TN	2021RUS
		325.40	g	u	-1678.8	5.9	-73.3	5.9			R	2019DIK
		325.40	l	u	-1647.9	5.9	-104.2	5.9	30.91	0.29	R	2019DIK
		325.40	l		-1632.2		-119.9				C	1920MOU
Ketones												
C_3H_6O	acetone	329.22	l	SEL	-1789.79	0.35	-248.12	0.35	31.38	0.10	TN	2021RUS
		329.22	g	SEL1	-1821.17	0.35	-216.74	0.35			TN	2021RUS
		329.22	g		-1821.3	2.1	-216.6	2.1			R	2019DIK
		329.22	g		-1819.41	0.59	-218.50	0.59			LiB	1991WIB
		329.22	g		-1820.8	0.5	-217.1	0.5			R	1976CHA
		329.22	g		-1820.38	0.67	-217.53	0.67			E	1965BUC
		329.22	g		-1821.5		-216.4					1957PEN
		329.22	g		-1821.40	0.84	-216.51	0.84			C	1941MIL
		329.22	l		-1790.1	2.1	-247.8	2.1	31.18	0.39	R	2019DIK
		329.22	l		-1788.54	0.63	-249.37	0.63	30.84		LiB	1991WIB
		329.22	l		-1771.5		-266.4				C	1918GUI
		329.22	l		-1804.2		-233.7				C	1911EME
		329.22	lg						31.30			1975AMB
		329.22	lg						29.66	0.01		1926MAT
C_4H_8O	butanone	352.74	l	SEL	-2443.83	0.79	-273.38	0.79	34.92	0.10	TN	2021RUS
		352.74	g	SEL1	-2478.75	0.79	-238.46	0.79			TN	2021RUS
		352.74	g	u	-2477.8	6.7	-239.4	6.7			R	2019DIK
		352.74	l	u	-2442.9	6.7	-274.3	6.7	34.84	0.18	R	2019DIK
		352.74	g		-2478.64	0.84	-238.57	0.84			R	1976CHA
		352.74	g		-2478.51	0.96	-238.70	0.96			E	1965BUC
		352.74	l		-2444.2		-273.0		34.97		C	1964SIN

		352.74	l		-2438.4		-278.8				C	1950PAR
		352.74	l		-2436.3	1.5	-280.9				C	1942CRO
		352.74	lg						34.92		R	1985MAJ
		352.74	lg						34.80	0.10		1983UCH
		352.74	lg						35.51	0.08		1979SUN
		352.74	lg						31.97	0.10		1926MAT
Carboxylic Acids												
CH_2O_2	formic acid	374.05	l	SEL	-254.59	0.20	-424.71	0.20	46.33		TN	2021RUS
		374.05	g	SEL1	-300.92	0.22	-378.38	0.22			TN	2021RUS
		281.47	s	SEL2	-241.9	1.0	-437.4	1.0	12.68	1.00	DfusH	2021RUS
		374.05	g	u	-275	9	-405	9			R	2019DIK
		374.05	l		-254.45	0.85	-424.85	0.85	20.1	9.1	R	2019DIK
		374.05	l		-254.2		-425.1		46.48		H2O	1974GUT
		374.05	l		-253.80	0.30	-425.50	0.30			C	1964LEB
		374.05	l		-254.60	0.30	-424.70	0.30	46.30	0.50	C	1959SIN
		374.05	lg						36.00		R	1987STE
		281.47	lg						46.30		R	1985MAJ
		374.05	lg						46.30	0.50		1970KON
		374.05	lg						19.90			1941STO
		281.47	sl	SEL					12.68	1.00	f	1941STO
$C_2H_4O_2$	acetic acid	391.20	l	SEL	-874.95	0.18	-483.65	0.18	50.91	0.30	TN	2021RUS
		391.20	g	SEL1	-925.86	0.38	-432.74	0.38			TN	2021RUS
		289.70	s	SEL2	-863.23	0.35	-495.37	0.35			DfusH	2021RUS
		391.20	l		-874.72	0.83	-483.89	0.82			R	2019DIK
		391.20	l		-875.16	0.34	-483.44	0.34			C	1997STE
		391.20	l		-874.20	0.21	-484.40	0.21			C	1964LEB
		391.20	l		-874.46	0.42	-484.15	0.42			C	1959EVA
		391.20	lg						50.2			2000VER
		391.20	lg						50.3			2000VER
		391.20	lg						51.60	1.50		1970KON
		289.70	sl	SEL					11.72		f	1996DOM
C_3H_6O	propanoic acid	413.99	l	SEL	509.60	0.18	-509.60	0.18	55.36	0.20	TN	2021RUS
		413.99	g	SEL1	454.24	0.28	-454.24	0.28			TN	2021RUS
		413.99	g		-1558.23	0.88	-479.67	0.88			R	2019DIK
		413.99	l		-1527.17	0.59	-510.74	0.58	31.06	0.66	R	2019DIK
		413.99	l		-1527.29	0.13	-510.62	0.14			C	1964LEB
		413.99	l		-1528.0		-509.9				C	1935SCH

		413.99	lg						54.50			2000VER
		413.99	lg						54.40			2000VER
		413.99	lg						54.90			1995CHI
		413.99	lg						55.0	2.0		1970KON
		413.99	lg						30.63			1926MAT
C_4H_8O	n-butanoic acid	436.42	l	SEL	-2183.50	0.59	-533.70	0.59			C	1964LEB
		436.42	g	SEL1	-2241.73	0.43	-475.47	0.42			DvH	1964LEB
		436.42	g		-2224.2	2.7	-493.0	2.7			R	2019DIK
		436.42	l		-2183.3	1.3	-533.9	1.3	40.8	2.4	R	2019DIK
		436.42	lg	SEL					58.23	0.30	v	2000VER
		436.42	lg						58.10			2000VER
		436.42	lg						58.50			2000VER
		436.42	lg						60.70			1995CHI
		436.42	lg						58.0	4.0		1970KON
Esters												
$C_3H_6O_2$	ethyl formate	327.29	l	SEL	-1611.8	1.2	-426.1	1.2	32.10	0.15	TN	2021RUS
		327.29	g	SEL1	-1643.9	1.2	-394.0	1.2			TN	2021RUS
		327.29	g		-1639.3	8.4	-398.6	8.4			R	2019DIK
		327.29	l		-1607.4	8.4	-430.5	8.4	31.92	0.30	R	2019DIK
		327.29	l		-1643.7	0.8	-394.2	0.8			E	1991FRO
		327.29	l		-1607.4		-430.5				E	1974HIN
		327.29	lg						32.11		R	1985MAJ
		327.29	lg						32.17			1974HIN
		327.29	lg						32.50			1974HIN
		327.29	lg						30.12	0.10		1926MAT
$C_2H_4O_2$	methyl formate	305.14	l	SEL	-970.10	0.86	-388.50	0.86	28.58	0.20	TN	2021RUS
		305.14	g	SEL1	-998.68	0.84	-359.92	0.84			TN	2021RUS
		305.14	g		-1000.9	1.9	-357.7	1.9			R	2019DIK
		305.14	g		-996.3		-362.3				E	1974HIN
		305.14	l		-972.5	1.8	-386.1	1.8	28.37	0.43	R	2019DIK
		305.14	l		-992.7		-365.9				E	1990GLA
		305.14	l		-967.8		-390.8		28.37		E	1974HIN
		305.14	l		-980.6		-378.0				H2O	1974GUT
		305.14	l		-972.61	0.59	-385.99	0.59	30.59		C	1971HAL
		305.14	lg						28.60		R	1985MAJ
		305.14	lg						28.24	0.04		1926MAT
$C_4H_8O_2$	ethyl acetate	350.21	l	SEL	-2237.35	0.46	-479.86	0.46	35.15	0.21	H2O	1991WIB2

		350.21	g	SEL1	-2272.49	0.51	-444.72	0.51			H2O	1991WIB2
		350.21	g		-2273.73	0.80	-443.48	0.79			R	2019DIK
		350.21	l		-2238.39	0.75	-478.82	0.75	35.34	0.25	R	2019DIK
		350.21	l		-2236.63	0.80	-480.57	0.79			LiB	1991WIB
		350.21	l		-2238.54	0.48	-478.67	0.48			C	1978FEN
		350.21	l		-2235.4	3.9	-481.8	3.9			C	1970BUT
		350.21	l		-1350.5		-461.6				C	1929ROT
		350.21	l		-2246.4		-470.8				C	1918GUI
		350.21	lg						35.00			1995CHI
		350.21	lg						35.60	0.10		1980SVO
		350.21	lg						35.15	0.21		1966WAD
		350.21	lg						32.30	0.42		1926MAT
$C_4H_6O_2$	vinyl acetate	345.33	l	SEL	-2080.6	2.0	-350.8	2.0	37.15	0.84	H2	1980VIL
		345.33	g	SEL1	-2117.7	2.2	-313.6	2.2			DvH	1980VIL
		345.33	l	u	-2086	10	-346	10			C	1980VIL
		345.33	g		-2116.6	2.8	-314.8	2.8			R	2019DIK
		345.33	l		-2081.5	2.8	-349.9	2.8	35.12	0.35	R	2019DIK
$C_5H_8O_2$	ethyl acrylate	372.59	l	SEL	-2740.1		-370.6				H2	1980VIL
		372.59	g	SEL1	-2779.3		-331.4				DvH	1980VIL
		372.59	g		-2773.2	2.8	-337.5	2.8			R	2019DIK
		372.59	l		-2734.1	2.8	-376.6	2.8			R	2019DIK
		372.59	l		-2715.0		-395.6		39.20		C	1975VIL
		372.59	l		-2743.3		-367.4				C	1972BAR
		372.59	lg	SEL					39.20		v	1975VIL
	methyl methacrylate	369.73	l	SEL	-2728.3	4.0	-382.4	4.0				1980VIL
		369.73	g	SEL1	-2768.3	4.0	-342.3	4.0				1980VIL
		369.73	g		-2775.11	0.78	-335.58	0.78			R	2019DIK
		369.73	l		-2735.60	0.74	-375.09	0.74	39.51	0.25	R	2019DIK
		369.73	l		-2724.6	4.0	-386.1	4.0			C	1980VIL
		369.73	lg						40.08			1975VIL
Oxacyclohydrocarbons												
C_2H_4O	oxirane	283.59	g	SEL	-1306.00	0.37	-52.60	0.37			TN	2021RUS
		283.59	l	SEL1	-1281.07	0.44	-77.53	0.44	24.93	0.24	TN	2021RUS
		283.59	g		-1306.8	2.0	-51.8	2.0			R	2019DIK
		283.59	g		-1306.04	0.59	-52.57	0.59			C	1965PEL
		283.59	g		-1307.71	0.84	-50.89	0.84			C	1942CRO
		283.59	l		-1281.8	2.0	-76.8	2.0	24.93	0.24	R	2019DIK

		283.59	l		-1262.9	1.3	-95.7	1.3			C	1937MOU
		283.59	lg						25.90		R	1987STE
		283.59	lg						25.51		R	1985MAJ
C_4H_4O	furan	304.51	l	SEL	-2083.5	0.6	-62.0	0.6	27.60	0.20	C	1952GUT
		304.51	g	SEL1	-2111.1	0.6	-34.4	0.6			DvH	1952GUT
		304.51	g		-2110.76	0.86	-34.80	0.86			R	2019DIK
		304.51	g		-2117.9		-27.7					1991ZAH
		304.51	l		-2083.34	0.85	-62.21	0.84	27.41	0.18	R	2019DIK
		304.51	l		-2088.2		-57.3				C	1929LAN
		304.51	lg						27.71		R	1985MAJ
		304.51	lg						28.20			1970MOI
$C_3H_6O_3$	1,3,5-trioxane	335.65	s	SEL	-1515.70	0.30	-522.21	0.30			C	1969MAN
		387.20	l	SEL1	-1526.4	4.8	-511.5	4.8			DfusH	1969MAN
		387.20	g	SEL2	-1572.3	0.5	-465.6	0.5			DsubH	1969MAN
		387.20	g		-1571.78	0.62	-466.13	0.62			R	2019DIK
		387.20	l		-1525.4	5.6	-512.5	5.6	46.3	4.9	DvH	2019DIK
		335.65	s	SEL	-1514.7	0.5	-523.2	0.5	10.73	0.20	f	2019DIK
		335.65	s		-1513.0	0.4	-524.9	0.4			C	1971HAY
		335.65	s		-1492.0	1.0	-545.9	1.0			C	1943WAL
		335.65	s		-1518.0		-519.9				C	1942DEL
		335.65	sg						57.06	0.37	R	2019DIK
		387.20	sg						55.6			1983WIT
		387.20	sg	SEL					56.60	0.20	s	1969MAN
		387.20	sg						48.5	2.5		1943WAL
$C_4H_8O_2$	1,3-dioxane	378.13	l	SEL	-2339.86	0.99	-377.35	0.99	39.09	0.05	C	1982BYS
		378.13	g	SEL1	-2378.95	0.99	-338.26	0.99			DvH	1982BYS
		378.13	g		-2372.5	5.6	-344.7	5.6			R	2019DIK
		378.13	l		-2333.8	5.4	-383.4	5.4	38.69	1.60	R	2019DIK
		378.13	l		-2339.86	0.99	-377.35	0.99			C	1982MOS
		378.13	l		-2332.8	1.8	-384.4	1.8			C	1968PIH
		378.13	l		-2331.8	0.8	-385.4	1.8			C	1968PIH
		378.13	l		-2331.91	0.84	-385.30	0.84	35.00	1.91	C	1967PIH
		378.13	l		-2340.82	0.59	-376.39	0.59	35.60		C	1961SNE
		378.13	l		-2322.1		-395.1		35.56	0.84	C	1959FLE
		378.13	l		-2331.32	0.84	-385.88	0.84			C	1957SKU
	1,4-dioxane	374.25	l	SEL	-2362.23	0.99	-354.98	0.99	38.64	0.05	C	1982BYS
		374.25	g	SEL1	-2362.28	0.99	-354.93	0.99			DvH	1982BYS

		374.25	g		-2402.1	2.2	-315.1	2.2			R	2019DIK
		374.25	g		-2399.4	1.7	-317.8	1.7			DvH	1961SNE
		374.25	l		-2363.4	2.2	-353.8	2.2	38.73	0.39	R	2019DIK
		374.25	l		-2363.9	0.5	-353.3	0.5	35.50	1.60	C	1961SNE
		374.25	l		-2346.2		-371.0				C	1933ROT
		374.25	l		-2186.8		-530.4				C	1929HER
		374.25	lg						39.80			1982BYS
		374.25	lg						34.10			1957GLA
		374.25	lg						37.49			1938CRE
$C_{10}H_{16}O$	D-camphor	451.8	s	SEL	-5902.0	3.0	-319.4	3.0			C	1977STE
		493.00	g	SEL1	-5953.9	3.1	-267.5	3.1			DsubH	1977STE
		451.8	l	SEL2	-5908.8	3.2	-312.5	3.2			DvH	1977STE
		451.8	sg	u					59	23	R	2019DIK
		493.00	lg						55.30	na		2002ROO
		493.00	lg	SEL					6.82		v	1995CHI
		451.8	s		-5891.2		-330.2				C	1932SHC
		451.8	s		-5898.6	3.8	-322.8	3.8			C	1929SWI
		451.8	s		-5910.7		-310.7				C	1913ROT
		451.8	sg						54.40			1995CHI
		451.8	sg						54.50			1995CHI
		451.8	sg						55.20			1995CHI
		451.8	sg	SEL					51.88	0.84	s	1977STE
$C_4H_2O_3$	2,5-furandione	325.65	s	SEL	-1389.50	0.67	-470.23	0.67			C	1964WIL
		478.33	g	SEL1	-1458.5	2.1	-401.2	2.1			DvH	1964WIL
		478.33	l	SEL2	-1401.0	2.1	-458.8	2.1			DfusH	1964WIL
		478.33	g		-1458.0	2.3	-401.8	2.3			R	2019DIK
		478.33	l	SEL	-1400	10	-459	10	57.5	9.5	v	2019DIK
		325.65	s	SEL	-1389.8	1.1	-470.0	1.1	10.68		f	2019DIK
		325.65	s		-1390.30	0.71	-469.43	0.71			C	1950PAR
		325.65	sg						68.2	2.0	R	2019DIK
		325.65	sg						70.0	2.0		1978VIL
Aromatic Alcohols												
C_6H_6O	phenol	314.15	s	SEL	-3055.98	0.65	-162.35	0.65	69.01	0.30	TN	2021RUS
		454.91	g	SEL1	-3124.99	0.63	-93.34	0.63			TN	2021RUS
		454.91	l	SEL2	-3071.06	0.70	-147.28	0.70			DfusH	2021RUS
		454.91	g		-3122.5		-95.9				R	2019DIK
		454.91	g		-3121.98	0.59	-96.36	0.59			DsubH	1961COX

		454.91	g		-3121.89	0.63	-96.44	0.63			C	1960AND
		454.91	l		-3068.4	2.8	-149.9	2.8	58.34	1.04	R	2019DIK
		314.15	lg						58.8			1995CHI
		314.15	s		-3053.32	0.68	-165.01	0.67	15.07		DfusH	2019DIK
		314.15	s		-3053.6	0.3	-164.7	0.3			C	1961COX
		314.15	s		-3053.50	0.67	-164.83	0.67			C	1960AND
		314.15	s		-3055.8		-162.5				C	1954PAR
		314.15	s		-3054.7		-163.6				C	1941BAD
		314.15	sg						69.14	0.49	R	2019DIK
		314.15	sg						69.70	0.90		1971PAR
		314.15	sg						68.6			1961'COX
		314.15	sg						68.66	0.50		1960AND
C_7H_8O	3-methylphenol	475.28	l	SEL	-3703.89	0.59	-193.75	0.59	61.71	1.05	C	1960AND
		475.28	g	SEL1	-3765.6	1.2	-132.0	1.2			DvH	1960AND
		285.37	s	SEL2	-3693.18	0.78	-204.46	0.78			DfusH	1960AND
		475.28	g		-3769.9	4.0	-127.7	4.0			R	2019DIK
		475.28	l		-3704.11	1.15	-193.53	1.15	65.8	3.8	R	2019DIK
		475.28	l		-3704.68	0.25	-192.96	0.26	59.70		C	1961COX
		475.28	l		-3721.2		-176.4				C	1954PUS
		475.28	l		-3704.4		-193.2				C	1941BAD
		475.28	l		-3694.5		-203.2				C	1925BAR
		475.28	lg						65.00	0.70		2007RIC
		475.28	lg						62.50			1995CHI
		475.28	lg						61.70		R	1987STE
		475.28	lg						61.70			1958BID
		475.28	lg						46.28			1957GLA
		285.37	sg						56.10		R	1987STE
		285.37	sl	SEL					10.71		f	1996DOM
	benzyl alcohol	478.50	l	SEL	-3736.9	1.3	-160.7	1.3			C	1954PAR
		478.50	g	SEL1	-3801.7	1.4	-95.9	1.4			DvH	1954PAR
		478.50	g	u	-3776.7	5.8	-120.9	5.8			R	2019DIK
		478.50	l	u	-3711.5	6.1	-186.1	6.1	65.17	1.94	R	2019DIK
		478.50	l	u	-3723.3		-174.3				C	1929LAN
		478.50	l	u	-3723.8		-173.9				C	1925BAR
		478.50	l		-3743.0	2.8	-154.6	2.8	60.30	0.30	C	1995PAP
		478.50	l		-3731.3		-166.3				C	1906SCH
		478.50	lg						65.50	0.40		2005VAS

		478.50	lg	SEL					64.80	0.60	v	1999VER
		478.50	lg						69.50			1995CHI
		478.50	lg						62.50	0.30		1990AMB
		478.50	lg						62.10	0.30		1949DRE
		478.50	lg						63.0	2.2		1937GAR
		478.50	lg						60.29	0.42		1926MAT
Oxa-Aromatics												
C_7H_6O	benzaldehyde	451.15	l	SEL	-3525.01	1.10	-86.80	1.10	49.73	0.40	TN	2021RUS
		451.15	g	SEL1	-3574.74	0.91	-37.07	0.91			TN	2021RUS
		451.15	g		-3576.1	5.4	-35.8	5.4			R	2019DIK
		451.15	g		-3578.5		-33.3					1975KUD
		451.15	g		-3574.6	4.2	-37.2	4.2				1971SOL
		451.15	l		-3526.0	5.4	-85.8	5.4	50.01	0.40	R	2019DIK
		451.15	l		-3525.0	2.0	-86.8	2.0	50.30		C	1975AMB
		451.15	l		-3528.79	0.84	-83.02	0.84	49.79	0.84	C	1972LEB
		451.15	l		-3525.9		-86.0				C	1929LAN
		451.15	lg						49.00	0.70		2007EME
		451.15	lg						49.10			1995CHI
		451.15	lg						45.90			1972LEB
		451.15	lg						40.92			1957GLA
$C_7H_6O_2$	benzoic acid	395.50	s	SEL	-3227.01	0.18	-384.80	0.17			TN	2021RUS
		523.53	g	SEL1	-3317.62	0.21	-294.19	0.20	90.61	0.50	TN	2021RUS
		523.53	l	SEL2	-3238.72	0.21	-373.09	0.20			DvH	2021RUS
		523.53	g		-3318.7	1.4	-293.1	1.4			R	2019DIK
		523.53	g		-3316.30	0.54	-295.51	0.54			DsubH	1969GUN
		523.53	lg	SEL					78.90		v	1995CHI
		395.50	s		-3227.7	1.4	-384.1	1.4			R	2019DIK
		395.50	s		-3228.06	0.44	-383.75	0.44		_	C	1984PIL
		395.50	s		-3226.87	0.18	-384.94	0.18		_	C	1969MOS
		395.50	s		-3227.0	0.2	-384.8	0.2			C	1969GUN
		395.50	s		-3228.0	0.5	-383.8	0.5		_	C	1960LI
		395.50	s		-3227.30	0.30	-384.51	0.30		_	C	1960COR
		395.50	s		-3227.40	0.30	-384.41	0.30		_	C	1958GUN
		395.50	s		-3227.2	0.5	-384.6	0.5		_	C	1956COO
		395.50	s		-3227.30	0.30	-384.51	0.30		_	C	1955CHA
		395.50	s		-3227.51	0.32	-384.30	0.32		_	C	1946JES
		395.50	s		-3227.60	0.30	-384.21	0.30		_	C	1944PRO

	395.50	s		-3226.39	0.32	-385.42	0.32		_	C	1942JES
	395.50	s		-3229.8		-382.0			_	C	1939MAT
	395.50	s		-3228.8		-383.0			_	C	1934HIR
	395.50	s		-3231.3		-380.5			_	C	1932MIL
	395.50	s		-3229.0		-382.8			_	C	1931BUR
	395.50	s		-3226.0		-385.8			_	C	1929LAN
	395.50	s		-3232.0		-379.8			_	C	1911WRE
	395.50	sg						91.04	0.14	R	2019DIK
	395.50	sg						93.30	1.20		2008FRE
	395.50	sg						90.40	0.50		2006RIB
	395.50	sg						88.30	0.50		2001KIY
	395.50	sg	SEL					89.30	0.50	s	1990SIL
	395.50	sg						89.23	0.50		1990SIL
	395.50	sg						89.01	0.33		1973MAL
	395.50	sg						86.6			1972WIE
	395.50	sg						89.50	0.20		1972MOR
	395.50	sg						89.70	0.60		1969CHA
	395.50	sg						91.40	0.40		1954DAV

NITROGEN-SUBSTITUTED HYDROCARBONS												
Hydrogen Cyanide												
CHN	hydrogen cyanide	298.79	l	SEL	-639.08	0.30	102.69	0.30			DvH	2021RUS
		298.79	g	SEL1	-665.669	0.092	129.280	0.089			TN	2021RUS
		298.79	g	SEL	-665.4	2.7	129.0	2.7	26.59	0.29	v	2019DIK
		298.79	l		-638.8	2.7	102.4	2.7			R	2019DIK
Alkylamines												
CH_5N	methylamine	266.84	g	SEL	-1086.81	0.24	-21.23	0.24			TN	2021RUS
		266.84	l	SEL1	-1062.79	0.45	-45.25	0.45	24.02	0.30	TN	2021RUS
		266.84	l	u	-1093.7		-14.3				C	1910MUL
		266.84	g		-1085.6	2.7	-22.4	2.7			R	2019DIK
		266.84	g		-1086.28	0.86	-21.76	0.86			E	1960ISS
		266.84	l		-1060.75	0.95	-47.29	0.94	23.76	0.28	R	2019DIK
		266.84	l		-1060.81	0.38	-47.23	0.38			C	1937AST
		266.84	lg						23.85		R	1985MAJ
C_2H_7N	ethylamine	289.79	g	SEL	-1737.31	0.54	-50.03	0.54			TN	2021RUS
		289.79	l	SEL1	-1713.25	0.55	-74.09	0.55	24.06		TN	2021RUS
		289.79	g		-1739.8	1.4	-47.5	1.4			R	2019DIK
		289.79	l		-1713.1	1.3	-74.3	1.3	26.76	0.44	R	2019DIK
		289.79	l		-1715.0		-72.3				C	1907LEM
		289.79	lg						27.00	0.50		1970COX
C_3H_9N	1-propylamine	320.38	l	SEL	-2365.13	0.41	-101.52	0.41	31.42	0.15	TN	2021RUS
		320.38	g	SEL1	-2396.55	0.42	-70.10	0.42			TN	2021RUS
		320.38	g		-2396.42	0.61	-70.23	0.61			R	2019DIK
		320.38	g		-2396.77	0.84	-69.87	0.84			R	1971SCO
		320.38	l		-2365.14	0.58	-101.51	0.57	31.28	0.21	R	2019DIK
		320.38	l		-2365.3	2.9	-101.4	2.9	31.34	0.21	C	1967SMI
		320.38	lg						31.30			1979MAJ2
		320.38	lg						29.20			1957GLA
	isopropylamine	304.92	l	SEL	-2354.37	0.52	-112.28	0.52	28.71	0.20	TN	2021RUS
		304.92	g	SEL1	-2383.08	0.53	-83.57	0.53			TN	2021RUS
		304.92	g		-2382.9	0.8	-83.7	0.8			R	1971SCO
		304.92	l		-2354.50	0.50	-112.15	0.71	28.50	0.20	C	1967SMI
$C_4H_{11}N$	n-butylamine	350.12	l	SEL	-3018.46	1.13	-127.48	1.13	32.64	1.26	C	1959EVA
		350.12	g	SEL1	-3054.17	1.13	-91.77	1.13			DvH	1959EVA
		350.12	g		-3054.22	1.32	-91.73	1.32			R	2019DIK
		350.12	l		-3018.31	1.30	-127.64	1.30	35.91	0.25	R	2019DIK

		350.12	lg						36.00			1995WOL
		350.12	lg						35.60			1995CHI
		350.12	lg						35.70	0.20		1985KUS
		350.12	lg						35.70	0.10		1979MAJ2
		350.12	lg	SEL					35.71	0.06	v	1969WAD
		350.12	lg						27.15			1957GLA
C_2H_7N	dimethylamine	280.02	g	SEL	-1769.79	0.42	-17.55	0.42			TN	2021RUS
		280.02	l	SEL1	-1743.91	0.37	-43.43	0.37	25.88	0.20	TN	2021RUS
		280.02	g		-1767.8	2.1	-19.5	2.1			R	2019DIK
		280.02	l		-1743.44	0.68	-43.90	0.68	24.65	0.36	R	2019DIK
		280.02	l		-1743.51	0.42	-43.83	0.42	25.40	0.04	C	1960ISS
		280.02	l		-1750.0		-37.3				C	1907LEM
		280.02	lg						26.00			1960ISS
		280.02	lg						26.48	0.13		1939AST
C_3H_9N	methylethylamine	305.60	l	SEL	-2391.4	2.3	-75.2	2.3			TN	2021RUS
		305.60	g	SEL1	-2420.7	1.1	-45.9	1.1			TN	2021RUS
		305.60	g		-2421.1	2.7	-45.6	2.7			R	2019DIK
		305.60	l		-2392.1	2.8	-74.5	2.8	28.99	0.51	R	2019DIK
	trimethylamine	276.00	g	SEL	-2439.91	0.76	-26.74	0.76			TN	2021RUS
		276.00	l	SEL1	-2417.80	0.87	-48.85	0.87	22.11	0.10	TN	2021RUS
		276.00	g		-2442.92	0.76	-23.72	0.75			R	2019DIK
		276.00	g		-2442.92	0.76	-23.72	0.75			DvH	1960ISS
		276.00	l		-2420.90	0.63	-45.74	0.62	21.68	0.27	R	2019DIK
		276.00	l		-2421.03	0.63	-45.62	0.63			C	1970COX
		276.00	l		-2420.92	0.71	-45.73	0.71	22.01	0.08	E	1960ISS
$C_6H_{15}N$	triethylamine	361.93	l	SEL	-4377.09	0.54	-127.46	0.55			C	1966LEB
		361.93	g	SEL1	-4412.49	0.59	-92.06	0.58			DvH	1966LEB
		361.93	g		-4411.0	4.3	-93.6	4.3			R	2019DIK
		361.93	l		-4376.3	4.3	-128.3	4.3	34.72	0.30	R	2019DIK
		361.93	l		-4335.1		-169.5				C	1972BAR
		361.93	lg	SEL					35.40	0.20	v	2009MOK
		361.93	lg						35.50		R	1987STE
		361.93	lg						34.80	0.20		1979MAJ2
		361.93	lg						35.10			1975CHU
		361.93	lg						34.94	0.06		1969WAD
$C_6H_{13}N$	cyclohexylamine	406.98	l	SEL	-4071.3	1.3	-147.4	1.3			C	1979STE
		406.98	g	SEL1	-4113.8	1.3	-104.9	1.3			DvH	1979STE

		406.98	g		-4115.7	3.0	-103.1	3.0			R	2019DIK
		406.98	l		-4071.2	2.8	-147.6	2.8	44.51	0.98	R	2019DIK
		406.98	l		-4077.5	1.6	-141.2	1.6			C	1982GUT
		406.98	lg	SEL					42.80	0.10	v	1975BER
Alkanenitriles												
C_2H_3N	ethanenitrile	355.05	l	SEL	-1256.29	0.22	40.60	0.22	33.45	0.21	TN	2021RUS
		355.05	g	SEL1	-1289.74	0.25	74.05	0.25			TN	2021RUS
		355.05	l	u	-1247.2	7.2	31.5	7.2			C	1971HAL
		355.05	g		-1289.30	1.06	73.61	1.06			R	2019DIK
		355.05	l		-1256.28	0.94	40.59	0.94	33.02	0.49	R	2019DIK
		355.05	l		-1256.33	0.30	40.64	0.30	33.02	0.49	C	1983AN
		355.05	l		-1271.9		56.2				C	1909LEM
		355.05	lg						33.00			2004CHI
		355.05	lg						33.00			2004ANT
		355.05	lg						33.45	0.21		1983AN
		355.05	lg						32.94	0.06		1970HOW
C_3H_5N	propanenitrile	370.73	l	SEL	-1910.62	0.54	15.63	0.55	35.98		C	1971HAL
		370.73	g	SEL1	-1946.60	0.62	51.61	0.62			C	1971HAL
		370.73	g		-1947.0	1.8	52.0	1.8			R	2019DIK
		370.73	l		-1910.5	1.8	15.5	1.8	36.44	0.34	R	2019DIK
		370.73	l		-1918.4		23.4				C	1909LEM
		370.73	lg						37.10	0.30		2004CHI
		370.73	lg						37.10	0.30		2004ANT
		370.73	lg						36.03	0.02		1970HOW
		370.73	lg						36.70	0.30		1933HEI
C_4H_7N	butanenitrile	390.77	l	SEL	-2568.68	0.92	-5.61	0.92	36.99		C	1959EVA
		390.77	g	SEL1	-2605.67	0.92	31.37	0.95			DvH	1959EVA
		390.77	l		-2568.5	1.1	-5.8	1.1			R	2019DIK
		390.77	l		-2608.33	1.14	34.03	1.14			R	2019DIK
		390.77	l		-2578.6		4.3				C	1909LEM
		390.77	lg						39.20	0.10		1982FUC
		390.77	lg						39.33	0.08		1970HOW
		390.77	lg						40.50	0.20		1933HEI
C_3H_3N	propenenitrile	351.13	l	SEL	-1756.40	0.42	147.23	0.42	32.64		C	1971HAL
		351.13	g	SEL1	-1789.04	0.72	179.87	0.72			DvH	1971HAL
		351.13	g		-1790.4	4.2	181.2	4.2			R	2019DIK
		351.13	l		-1757.1	4.1	148.0	4.1	33.24	0.70	R	2019DIK

		351.13	l		-1749.3		140.2				C	1972BAR
		351.13	l		-1759.4	2.9	150.2	2.9	32.64		C	1945DAV
		351.13	lg						31.60		R	1987STE
Azahydrocarbons												
C_2N_2	cyanogen	252.00	g	SEL	-1097.07	0.41	310.12	0.41			TN	2021RUS
		252.00	l	SEL1	-1076.13	0.42	289.18	0.42	20.94		TN	2021RUS
		252.00	g		-1094.1	2.5	307.1	2.5			R	2019DIK
		252.00	g		-1096.0	1.8	309.0	1.8			C	1951KNO
		252.00	g		-1093.70	0.84	306.75	0.84			C	1933WAR
		252.00	g		-1051.9	5.0	264.9	5.0			C	1933MCM
		252.00	l		-1072.3	2.8	285.4	2.8	21.73	1.24	R	2019DIK
		252.00	lg						20.8		R	1985MAJ
$C_2H_8N_2$	1,1-dimethylhydrazine	335.57	l	SEL	-1978.7	3.6	48.4	3.6			C	1960DON
		335.57	g	SEL1	-2013.7	3.6	83.4	3.6			DvH	1960DON
		335.57	g		-2014.2	2.7	83.9	2.7			R	2019DIK
		335.57	l		-1979.2	2.5	48.9	2.5	35.02	0.76	R	2019DIK
		335.57	l		-1979.7	2.9	49.4				C	1952AST
		335.57	l	SEL					35.00	0.17	v	1952AST
$C_3H_6N_6$	1,3,5-triazine-2,4,6-triamine	618	s	SEL	-1972.0	3.0	-65.9	3.0			C	1973SEL
		618	s		-1966.24	0.53	-71.67	0.53			R	2019DIK
		618	s		-1951.0		-86.9				C	1972BAR
		618	s		-1966.4	2.0	-71.5	2.0			C	1956HAV
		618	s		-1966.5		-71.4				C	1955SAL
C_6H_7N	aniline	457.30	l	SEL	-3393.06	0.84	31.81	0.84	55.77		C	1962HAT
		457.30	g	SEL1	-3448.27	0.88	87.03	0.88			DvH	1962HAT
		457.30	g		-3447.6	2.1	86.4	2.1			R	2019DIK
		457.30	l		-3392.6	1.7	31.3	1.7	55.04	1.20	R	2019DIK
		457.30	l		-3392.0		30.7		52.72		C	1952VRI
		457.30	l		-3392.3		31.1				C	1951COL
		457.30	l		-3391	13	30		50.21		C	1942AND
		457.30	lg						55.83	0.02		1971KUS
$C_8H_{11}N$	*N*,*N*-dimethylaniline	466.47	l	SEL	-4767.8	3.2	47.9	3.2	52.83	0.03	C	1982FUR
		466.47	g	SEL1	-4820.6	3.2	100.8	3.2			DvH	1982FUR
		275.65	s	SEL2	-4756.2	3.2	36.4	3.2			DfusH	1982FUR
		466.47	g		-4819.5	3.0	99.7	3.0			R	2019DIK
		466.47	l		-4766.2	2.6	46.3	2.6	53.37	1.42	R	2019DIK
		466.47	l		-4754.3		34.4		49.79		C	1952VRI

		275.65	sl	SEL					11.56		f	1972AHN
$C_6H_{15}NO_3$	triethanolamine	623.15	l	SEL	-3840.6	1.5	-664.0	1.5	105.9	2.2	C	1982MIN
		623.15	g	SEL1	-3946.3	2.7	-558.3	2.7			DvH	1982MIN
		623.15	g	u	-3941	26	-563	26			R	2019DIK
		623.15	l		-3840.4	2.9	-664.2	2.9	101	26	R	2019DIK
Nitroalkanes and Nitrites												
CH_3NO_3	methyl nitrate	338.00	g	SEL	-700.0	1.3	-122.2	1.3			E	1959RAY
		338.00	g		-700.0	2.5	-122.2	2.5			R	2019DIK
		338.00	l		-672.4	2.9	-149.8	2.9	27.63	1.46	R	2019DIK
		338.00	lg						34.10			1957GRA
CN_4O_8	tetranitromethane	397.95	l	SEL	-431.8	1.7	38.3	1.7	43.93	0.42	C	1975LEB
		397.95	g	SEL1	-475.7	1.7	82.2	1.7			DvH	1975LEB
		287.05	s	SEL2	-395.4	4.3	1.9	4.3			DfusH	1975LEB
		397.95	l		-432.7	3.1	39.2	3.1			R	2019DIK
		397.95	l		-430.3	2.9	36.8	2.9			C	1963GAR
		397.95	l		-434.7	4.2	41.2	4.2			C	1944ROT
		287.05	sl	SEL					36.4	4.0	f(est)	2021CHE
CH_3NO_2	nitromethane	374.34	l	SEL	-709.25	0.43	-112.97	0.43	38.26	0.10	TN	2021RUS
		374.34	g	SEL1	-747.51	0.46	-74.71	0.46			TN	2021RUS
		374.34	g		-749.9	3.5	-72.3	3.5			R	2019DIK
		374.34	l		-711.4	3.5	-110.8	3.5	38.46	0.30	R	2019DIK
		374.34	l		-712.51	0.55	-109.71	0.55			C	1973LEB
		374.34	l		-709.61	0.42	-112.61	0.42			C	1973LEB
		374.34	l		-702.91	1.26	-119.30	1.26			C	1971KNO
		374.34	l		-709.23	0.59	-112.99	0.59			C	1958CAS
		374.34	l		-733.25	0.75	-88.97	0.75	38.03	0.38	C	1949HOL
		374.34	l		-709.2		-113.0				C	1910SWI
		374.34	lg						37.20			1995CHI
		374.34	lg						38.37			1954MCC
		374.34	lg						38.30	0.10		1947JON
		374.34	lg						34.48	0.08		1926MAT
$C_9H_6N_2O_2$	2,4-diisocyanatotoluene	524.83	l	SEL	-4235.0		-163.7		49.5		C	1962STR
		524.83	g	SEL1	-4284.5		-114.2				DvH	1962STR
		293.65	s	SEL2	-4168.0		-230.8				est	1985CHR
		524.83	lg	SEL					49.5	5.2	v	2019DIK
$C_6H_5NO_2$	nitrobenzene	483.81	l	SEL	-3082.0	1.4	6.6	1.4	55.00	0.05	TN	2021RUS
		483.81	g	SEL1	-3137.0	1.4	61.6	1.4			TN	2021RUS

		483.81	g		-3142.4	3.2	67.0	3.2			R	2019DIK
		483.81	l		-3087.4	2.9	11.9	2.9	55.03	1.37	R	2019DIK
		483.81	l		-3088.08	0.42	12.66	0.42	56.03	0.40	C	1971LEB
		483.81	l		-3095.7		20.3				C	1921GAR
		483.81	lg						54.50	na		1995CHI
		483.81	lg						56.10	1.70		1971LEB
		483.81	lg						55.01	0.02		1971KUS
$C_7H_5N_3O_6$	trinitrotoluene	355.10	s	SEL	-3406.0	3.0	-62.9	3.0			C	1976ROU
		621.00	g	SEL1	-3519.2	3.4	50.3	3.4			DsubH	1976ROU
		621.00	l	SEL2	-3493.0	3.6	24.1	3.6			DvH	1976ROU
		621.00	g		-3516.7	6.5	47.8	6.5			R	2019DIK
		621.00	g		-3493.0	3.5	24.1	3.5				1971LEN
		621.00	lg	SEL					87.00	1.90	v	1978CUN
		355.10	s		-3404.3	6.0	-64.6	6.0			R	2019DIK
		355.10	s		-3388.6	3.0	-80.3	3.0			C	1971LEN
		355.10	s		-3404.5	2.1	-64.4	2.1			C	1956YOU
		355.10	s		-3407.0		-61.9				C	1956HAN
		355.10	s		-3402.3	3.4	-66.6	3.4			C	1939BUR
		355.10	s		-3401.8	3.4	-67.1	3.4			C	1939BAD
		355.10	s		-3419.2		-49.7				C	1930RIN
		355.10	s		-3434.0		-34.9				C	1921GAR
		355.10	sg						112.4	2.6	R	2019DIK
		355.10	sg	SEL					113.20	1.50	s	1979KUD
		355.10	sg						104.60	1.70		1971LEN
		355.10	sg						118			1950EDW

SULFUR-SUBSTITUTED HYDROCARBONS													
Akanethiols													
CH_4S	methanethiol	279.05	g	SEL	-1544.57	0.51	-22.55	0.51			DvH		1961GOO
		279.05	l	SEL1	-1520.8	0.5	-46.35	0.5	23.81	0.08	R	a	1961GOO
		279.05	g		-1544.9	4.7	-22.2	4.7			R		2019DIK
		279.05	l		-1522.07	1.0	-45.04	1.01	23.51	0.94	R		2019DIK
		279.05	l		-1519.0	0.5	-46.7				C	e	1961GOO
		279.05	lg						23.80				1971WIL
C_2H_6S	ethanethiol	308.19	l	SEL	-2173.17	0.42	-73.68	0.42			C	a	1957MCC
		308.19	g	SEL1	-2200.3	0.43	-46.1	0.43			DvH		1957MCC
		308.19	g		-2199.7		-46.8	7.7			R		2019DIK
		308.19	l		-2172.5	7.7	-73.9	7.7	27.17	0.50	R		2019DIK
		308.19	l		-2172.00	0.42	-73.26	0.42	27.30	0.08	C	f	1957MCC
		308.19	l		-2164.0						C		1901BER
		308.19	lg						27.30				1971WIL
		308.19	lg						27.53				1957MCC
Sulfides													
CS_2	carbon disulfide	318.35	l	SEL	-1687.2	0.5	89.71				C	a	1961GOO
		318.35	g	SEL1	-1714.5	0.5	117.1				DvH		1961GOO
		318.35	g		-1716.10	1.24	118.66	1.24			R		2019DIK
		318.35	g		-1112.1						C		1949GUE
		318.35	l		-1688.61	1.23	91.17	1.23	27.50	0.15	R		2019DIK
		318.35	l		-1684.6	0.5	89.4		27.66	0.08	C	f	1961GOO
		318.35	lg						27.52	0.13			1962WAD
		318.35	lg						26.78	0.01			1926MAT
C_2H_6S	dimethyl sulfide	310.42	l	SEL	-2181.45	0.33	-64.96				C	a	1957MCC
		310.42	g	SEL1	-2208.8	0.59	-37.57	0.59			DvH		1957MCC
		310.42	g		-2208.4	7.7	-38.1	7.7			R		2019DIK
		310.42	l		-2180.8	7.7	-65.7	7.7	27.59	0.25	R		2019DIK
		310.42	l		-2181.0	1.5	-65.4	1.5	27.90	0.60			1989VOR
		310.42	l		-2180.24	0.33	-65.44		27.82	0.04	C	f	1957MCC
		310.42	l		-2186.2		-60.2						1946DOU
		310.42	lg						27.50				1981SHI
		310.42	lg						27.70				1971WIL
C_2H_6OS	dimethyl sulfoxide	463.86	l	SEL	-2037.30	1.25	-203.40		52.90	0.83	C	g	1994MAS
		463.86	g	SEL1	-2095.9	1.5	-150.5	1.5			DvH		1994MAS
		463.86	g		-2095.8	1.23	-150.64	1.23			R		2019DIK

	463.86	l	-2043.1	1.03	-203.30	1.03	52.66	0.68	R	2019DIK
	463.86	lg					52.89	0.42		1948DOU

HALOGENATED HYDROCARBONS													
Fluoroalkanes													
CH_3F	fluoromethane	194.65	g	SEL	-764.86	0.28	-235.49	0.23			TN	k	2021RUS
		194.65	l	SEL1	-756.33	1.15	-244.02	1.14			DvH		2021RUS
		194.65	g		-753.5		-246.9				R		1985LIA
		194.65	lg	SEL					8.53	1.12	v		2019DIK
CH_2F_2	difluoromethane	221.50	g	SEL	-584.82	0.40	-450.76	0.33			TN	k	2021RUS
		221.50	l	SEL1	-566.84	0.43	-468.74	0.36	17.98	0.20	TN		2021RUS
		221.50	g	u	-582.5	2.3	-453.0	2.3			R		2019DIK
		221.50	l	u	-568.6	2.3	-467.0	2.3	13.95	0.39	R		2019DIK
		221.50	g		-583.3	2.6	-452.3	2.6			CC		2019PAU
		221.50	g		-583.08	0.92	-452.21	0.92			C	j	1958NEU
CHF_3	trifluoromethane	188.75	g	SEL	-374.80		-696.00	0.41			TN	k	2021RUS
		188.75	l	SEL1	-366.34		-704.46	0.43	8.46	0.30	TN		2021RUS
		188.75	g	u	-390.5	2.7	-680.3	2.7			R		2019DIK
		188.75	l	u	-388.1	2.8	-682.7	2.7	2.42	0.32	R		2019DIK
		188.75	g		-372.5	2.7	-698.3	2.7			CC		2019PAU
		188.75	g		-374.2	2.8	-696.6	2.8			C	d	1958NEU
		188.75	g		-375.4	2.7	-695.4	2.7			C	b	1957NEU
CF_4	tetrafluoromethane	145.56	g	SEL	-172.55		-933.47	0.25			TN	k	2021RUS
		145.56	l	SEL1	-160.74		-945.28	0.56			DvH		2021RUS
		145.56	g	u	-185.1	5.9	-920.9	5.9			D		1961BAI
		145.56	g	u	-189	10	-917	10			C		1960VOR
		145.56	g	u	-197.7	5.0	-908.3	5.0			C		1957NEU
		145.56	g	u	-197.7	5.0	-908.3	5.0			C		1956NEU
		145.56	g	u	-191	17	-915	17			F2		1955JES
		145.56	g	u	-184	17	-922	17			F2		1955JES
		145.56	g	u	-194	17	-912	17			K		1954KIR
		145.56	g	u	-163	17	-943	17			K		1954KIR
		145.56	g	u	-193.9		-912.1						1954DUU
		145.56	g		-171.0	2.9	-935.0	2.9			CC		2019PAU
		145.56	g		-172.6	2.0	-933.4	1.9			R		2019DIK
		145.56	g		-173.0		-933.0				R		1979PRI
		145.56	g		-172.8		-933.2				R		1972WAL
		145.56	g		-172.82		-933.20	0.75			F2		1968GRE
		145.56	g		-171.7	1.7	-934.3	1.7			F2		1967WOO
		145.56	g		-173.54		-932.49	0.17			F2		1967DOM

		145.56	g		-178.4		-927.6				D		1965DOM
		145.56	g		-162.0	2.7	-944.0	2.7			R	a	1965COX
		145.56	g		-173.13	1.34	-914.46	1.34			R		1965COX
		145.56	g		-183.0	5.9	-923.0	5.9					1962BAI
		145.56	g		-158	10	-949	10					1960VOR
		145.56	g		-168.0	5.9	-938.1	5.9					1956NEU
		145.56	g		-173.6	4.2	-913.4	4.2			H2O		1956GOO
		145.56	g		-163.0	5.0	-943.1	5.0			H2O		1956GOO
		145.56	g		-173.6	4.2	-913.4	4.2			H2O		1955SCO
		145.56	g		-181.95	0.00	-924.08	0.00					1955SCO
		145.56	lg	SEL					11.81		v		1969SMI
C_2H_5F	fluoroethane	236.05	g	SEL	-1407.52	0.40	-272.13	0.36			TN		2021RUS
		236.05	l	SEL1	-1391.21	0.47	-288.45	0.44			DvH		2021RUS
		236.05	lg	SEL					16.32	0.25	v		2019DIK
$C_2H_4F_2$	1,1-difluoroethane	249.13	g	SEL	-1212.14	0.60	-502.74	0.55			DvH		2021RUS
		249.13	l	SEL1	-1193.66	0.88	-521.22	0.84			TN		2021RUS
		249.13	g	u	-1217	16	-498	16			R		2019DIK
		249.13	g	u	-1209	8	-505	8			G3B3		2016GOO
		249.13	g	u	-1219.6	8.4	-497.0	8.4			C		1968KOL
		249.13	l	u	-1199	16	-516	16	18.48	0.64	R		2019DIK
		249.13	g		-1210.9	2.1	-504.0	2.1			C		1968KOL
		249.13	l		-1210.3	2.6	-504.6	2.6			CC		2019PAU
	1,2-difluoroethane	293.00	g	SEL	-1267.04	0.84	-447.84	0.81			TN		2021RUS
		293.00	l	SEL1	-1245.91	0.98	-468.97	0.95	21.13	0.50	DvH		2021RUS
		293.00	g		-1267.3		-447.6				G3B3		2016GOO
		293.00	lg	SEL					21.13	0.50	v		2022BUR1
$C_2H_3F_3$	1,1,1-trifluoroethane	225.91	g	SEL	-1008.3	1.7	-748.5	1.7			C		1965KOL
		225.91	l	SEL1u	-988.2	2.0	-761.9	1.9			DvH		1965KOL
		225.91	g	u	-994	8	-756	8			G3B3		2016GOO
		225.91	lg	SEL					13.43	0.97	v		2019DIK
		225.91	g		-996.2	2.7	-753.9	2.7			CC		2019PAU
		225.91	g		-1001.4	3.2	-748.7	3.2			E		1974WU
	1,1,2-trifluoroethane	276.81	g	SEL	-1059	10	-691	10			H2		1965KOL
		276.81	l	SEL1	-1035	10	-715	10			DvH		1965KOL
		276.81	g		-1080.8	2.7	-669.3	2.7			CC		2019PAU
		276.81	g		-1053.8	3.0	-696.3	3.0			E		1956LAC
		276.81	lg	SEL					24.28	0.45	v		2019DIK

$C_2H_2F_4$	1,1,1,2-tetrafluoroethane	247.08	g	SEL	-883.7	2.0	-901.6	2.0			CBS		1988BER
		247.08	l	SEL1	-865.6	2.0	-919.7	2.0	18.10	0.16	DvH		1988BER
		247.08	lg	SEL					18.10	0.16	v		2019DIK
	1,1,2,2-tetrafluoroethane	253.23	g	SEL	-910.1	2.0	-875.2	2.0			CBS		1988BER
		253.23	l	SEL1	-890.3	2.3	-895.0	2.3			G3B3		2016GOO
		253.23	lg	SEL					19.79	1.13	v		2019DIK
C_2HF_5	pentafluoroethane	225.06	g	SEL	-701	8	-1120	8			G3B3		2016GOO
		225.06	l	SEL1	-687	8	-1133	8			DvH		2016GOO
		225.06	g		-705.2	3.1	-1115.4	3.1			CC		2019PAU
		225.06	lg	SEL					13.44	0.16	v		2019DIK
C_2F_6	hexafluoroethane	194.87	g	SEL	-513.33		-1342.44	0.97			TN		2021RUS
		194.87	l	SEL1	-506.33		-1349.44	1.09	7.00	0.50	DvH		2021RUS
		194.87	g	u	-588	8	-1268	8			R		2019DIK
		194.87	g	u	-524	8	-1331	8			E		1966SIN
		194.87	g		-510.0	3.3	-1345.8	3.3			CC		2019PAU
		194.87	g		-504.3		-1351.5				G3B3		2016GOO
		194.87	g		-511.9	5.0	-1343.9	5.0					1970WAL
		194.87	g		-525.3		-1330.5				E		1967COO
		194.87	g		-511.8	3.0	-1344.0	3.0			NF3	d	1966SIN
		194.87	g		-511.8	4.0	-1344.0	4.0			K	c	1954KIR
		194.87	lg	SEL					7.00	0.50	v		2022BUR1
Fluoroalkenes													
$C_2H_3F_3$	fluoroethene	201.65	g	SEL	-1251.41	0.48	-142.42	0.45			TN		2021RUS
		201.65	l	SEL1	-1240.61	0.90	-153.22	0.88			DvH		2021RUS
C_2H_3F		201.65	g		-1250.2	2.6	-143.6	2.6			CC		2019PAU
$C_2H_3F_3$		201.65	g		-1254.8	3.2	-139.0	3.2			R		2019DIK
C_2H_3F		201.65	g		-1256.0	1.7	-135.6	1.7			C		1970KOL
		201.65	g		-1255.1	1.9	-138.7	1.9			C	d	1970KOL
$C_2H_3F_3$		201.65	l	SEL	-1244.0	3.3	-149.8	3.3	10.80	0.76	v		2019DIK
$C_2H_2F_2$	1,1-difluoroethene	190.15	g	SEL	-1078.41	0.80	-350.64	0.77			TN		2021RUS
		190.15	l	SEL1	-1074.0	2.7	-355.1	2.7			DvH		2021RUS
		190.15	g	u	-1087	10	-344	10			C		1962KOL
		190.15	g		-1077.9	2.7	-351.2	2.7			CC		2019PAU
		190.15	g		-1094.9	3.4	-334.1	3.4			R		2019DIK
		190.15	g		-1104.0	3.4	-325.1	3.3			C		1957NEU
		190.15	g		-1097.0	3.4	-334.0	3.3			C		1956NEU
		190.15	lg	SEL	-1090.5	4.3	-338.6	4.3	4.4	2.6	v		2019DIK

	1,2-difluoroethene, (E)-	231.15	g	SEL	-1123.0	0.9	-306.1	0.9			TN		2021RUS
		231.15	l	SEL1	-1108.05	1.39	-321.00	1.38			DvH		2021RUS
		231.15	lg	SEL					14.90	1.04	v		2019DIK
	1,2-difluoroethene, (Z)-		g	SEL	-1119.4	0.9	-309.7	0.9			TN		2021RUS
		253.15	l	SEL1	-1105.6	1.3	-323.4	1.3			DvH		2021RUS
		253.15	lg	SEL					13.79	0.94	v		2019DIK
C_2HF_3	trifluoroethene	211.70	g	SEL	-966.2	1.6	-498.1	1.6			TN		2021RUS
		211.70	l	SEL1	-954.8	1.9	-509.5	1.8			DvH		2021RUS
		211.70	g	u	-971	21	-493	21			R		2019DIK
		211.70	g	u	-977	8	-474	8			C		1962KOL
		211.70	g		-965.5	2.8	-498.8	2.8			CC		2019PAU
		211.70	g		-977.9	3.9	-486.4	3.9			C	d	1962KOL
		211.70	lg	SEL					11.37	0.92	v		2019DIK
C_2F_4	tetrafluoroethene	197.51	g	SEL	-825.10	0.61	-674.40	0.52			TN		2021RUS
		197.51	l	SEL1	-819.00	1.44	-680.50	1.40			DvH		2021RUS
		197.51	g	u	-850	23	-650	23			R		2019DIK
		197.51	lg	SEL	-844	23	-656	23	6.10	1.30	v		2019DIK
		197.51	g		-826.3	3.0	-673.2	3.0			CC		2019PAU
		197.51	g		-839.4	5.5	-660.1	5.5			Na	d	1962KOL2
		197.51	g		-838.8	3.4	-660.7	3.3			Na		1962KOL
		197.51	g		-842.4	4.8	-657.1	4.8			H2	d	1956NEU
		197.51	g		-840.0	2.0	-659.5	2.0			D	d	1956NEU
		197.51	g		-838.8	3.4	-660.7	3.3			H2		1956NEU
		197.51	g		-787	10	-713	10			K	d	1955WAR
		197.51	g		-813.3		-686.2				K		1955WAR
		197.51	g		-823	7	-676	7			D	d	1955DUU
		197.51	g		-841.7	5.7	-657.8	5.7			H2	d	1955DUU
		197.51	g		-796	8	-704	8			K	d	1954KIR
		197.51	g		-821.7	4.2	-677.8	4.2			K		1954KIR
Chlorolakenes													
CH_3Cl	chloromethane	249.00	g	SEL	-763.51	0.39	-82.24	0.39			TN		2021RUS
		249.00	l	SEL1	-743.61	0.25	-102.14	0.25	19.90	0.30	TN		2021RUS
		249.00	g		-763.81	0.63	-81.94	0.63			R		2019DIK
		249.00	g		-763.9	1.5	-81.9	1.5			R		2002MAN
		249.00	g		-763.8	0.5	-82.0	0.5			C		1971FLE
		249.00	g		-759.7	0.6	-86.1	0.6			H2	b	1956LAC
		249.00	g		-759.86	0.59	-85.90	0.59			H2		1956LAC

		249.00	g		-760.4	0.6	-85.4	0.6			H2	b	1065FOW
		249.00	l		-743.4	1.5	-102.4	1.5	20.50	0.30	R		2002MAN
CH_2Cl_2	dichloromethane	312.92	g	SEL	-633.00	0.52	-93.38	0.52			TN		2021RUS
		312.92	l	SEL1	-603.99	0.54	-122.39	0.54	29.01	0.10	TN		2021RUS
		312.92	g		-631.0	0.4	-95.4	0.4			R		2019DIK
		312.92	g		-631.3	2.5	-95.1	2.5			R		2002MAN
		312.92	g		-602.5	0.8	-95.1	0.8			C	c	1969HU
		312.92	g		-630.4	1.3	-96.0	1.3			H2		1967LAC
		312.92	g		-630.69	1.34	-95.69	1.34			H2	b	1967LAC
		312.92	g		-634.6	8.4	-91.8	8.4			C	c	1938EFT
		312.92	l		-602.13	0.38	-124.25	0.38	28.88	0.13	R		2019DIK
		312.92	l		-602.3	2.5	-124.1	2.5	29.03	0.08	R		2002MAN
		312.92	l		-602.5		-124.3				C		1969HU
		312.92	l		-605.8	8.4	-120.6	8.4			C	b	1938EFT
		312.92	l		-604.6	8.4	-121.8	8.4			C		1938EFT
		312.92	lg						30.60	0.10			1989AN
		312.92	lg						28.80				1980HUG
		312.92	lg						28.45	0.42			1926MAT
$CHCl_3$	trichloromethane	334.42	g	SEL	-504.94	0.50	-102.07	0.50			TN		2021RUS
		334.42	l	SEL1	-473.54	0.51	-133.47	0.51	31.40	0.10	TN		2021RUS
		334.42	g		-503.8	1.7	-103.2	1.7			R		2019DIK
		334.42	g		-504.1	2.5	-102.9	2.5			R		2002MAN
		334.42	g		-502.0	1.4	-105.0	1.4			Br2	c	1973MEN
		334.42	g		-473.2		-96.2				C	c	1969HU
		334.42	g		-473.2	0.8	-102.9	0.8			C	c	1956KIR
		334.42	g		-504.9	8.4	-102.1	8.4			C	c	1938EFT
		334.42	l		-472.7	1.7	-134.3	1.7	31.12	0.31	R		2019DIK
		334.42	l		-472.9	2.5	-134.1	2.5	31.32	0.08	R		2002MAN
		334.42	l		-473.2	0.8	-134.3	0.8			C		1969HU
		334.42	l		-474.0	8.4	-133.0	8.4			C	b	1938EFT
		334.42	l		-473.4	8.4	-133.7	8.4			C		1938EFT
		334.42	lg						31.10				1980HUG
		334.42	lg						30.54	0.42			1926MAT
CCl_4	tetrachloromethane	349.65	g	SEL	-392.02	0.43	-95.61	0.43			TN		2021RUS
		349.65	l	SEL1	-359.52	0.43	-128.11	0.43	32.5		TN		2021RUS
		349.65	g		-391.69	1.31	-95.94	1.31			R		2019DIK
		349.65	g		-392.0	2.5	-95.6	2.5			R		2002MAN

		349.65	g		-393.9	1.7	-93.7	1.7			Br2		1973MEN
		349.65	g		-373.0	2.9	-114.6	2.9			D		1969LOR
		349.65	g		-362.9	4.6	-124.7	4.6			D		1969LOR
		349.65	g		-385	8	-103	8			D		1961BAI
		349.65	g		-394.1	1.4	-93.5	1.4			Br2	c	1937MEN
		349.65	l		-359.24	1.29	-128.39	1.29	32.45	0.22	R		2019DIK
		349.65	l		-359.5	2.5	-128.1	2.5	32.55	0.07	R		2002MAN
		349.65	l		-359.9		-128.4				C		1969HU
		349.65	l		-365.7	8.4	-121.9	8.4			C	b	1938EFT
		349.65	l		-365.2	8.4	-122.4	8.4			C		1938EFT
		349.65	lg						32.40				1980HUG
		349.65	lg						32.54	0.10			1973KON
		349.65	lg						32.43	0.01			1966WAD2
		349.65	lg						32.41	0.01			1959HIL1
		349.65	lg						29.96	0.01			1926MAT
C_2H_5Cl	chloroethane	285.40	g	SEL	-1413.57	0.26	-111.49	0.26			TN		2021RUS
		285.40	l	SEL1	-1389.14	0.40	-135.92	0.40	24.43	0.30	TN		2021RUS
		285.40	g	u	-1427	10	-100	10			C		1951CAS
		285.40	g		-1412.78	0.64	-112.28	0.64			R		2019DIK
		285.40	g		-1413.0	0.7	-112.1	0.7			R		2002MAN
		285.40	g		-1413.06	0.59	-112.26	0.59			C		1971FLE
		285.40	g		-1418.2	0.4	-106.9	0.4			H2	b	1956LAC
		285.40	g		-1417.36	0.59	-107.70	0.59			H2		1956LAC
		285.40	g		-1415.9	1.7	-109.2	1.7			HCl	b	1955HOW
		285.40	g		-1413.6	2.0	-111.5	2.0			HCl		1955HOW
		285.40	g		-1413.2	3.0	-111.9	3.0			HCl		1955HOW
		285.40	g		-1412.7	3.0	-112.4	3.0			HCl		1955HOW
		285.40	g		-1413.3		-111.7				HCl		1953LAN
		285.40	l		-1389.01	0.66	-136.05	0.66	23.77	0.15	R		2019DIK
		285.40	l		-1388.4	1.0	-136.7	1.0	24.60	0.30	R		2002MAN
$C_2H_4Cl_2$	1,1-dichloroethane	330.42	g	SEL	-1272.61	0.44	-133.07	0.44			TN		2021RUS
		330.42	l	SEL1	-1241.81	0.48	-163.87	0.48	30.8		TN		2021RUS
		330.42	g		-1273.2	3.5	-132.5	3.5			R		2002MAN
		330.42	g		-1274.2	3.5	-131.5	3.5			HCl	c	1976LEV
		330.42	g		-1273.2	3.5	-132.5	3.5			HCl	c	1976LEV
		330.42	g		-1272.5	3.5	-133.2	3.5			HCl	c	1976LEV
		330.42	g		-1278.07	1.13	-127.61	1.13			H2		1967LAC

		330.42	l		-1242.4	3.5	-163.3	3.5	30.83	0.08	R		2002MAN
		330.42	l		-1246.8	8.4	-158.9	8.4			C	b	1938EFT
		330.42	l		-1244.6	8.4	-161.1	8.4			C		1938EFT
		330.42	lg						30.73	0.15	R		2019DIK
		330.42	lg						30.62	0.14			1972LAY
	1,2-dichloroethane	356.70	l	SEL	-1238.5	3.5	-167.2	3.5	35.21	0.05	R		2002MAN
		356.70	g	SEL1	-1273.7	3.5	-132.0	3.5			R		2002MAN
		356.70	g		-1271.2	2.3	-134.5	2.3			R		2019DIK
		356.70	g		-1280.2	1.0	-125.4	1.0			H2	b	1967LAC
		356.70	g		-1279.4	1.0	-126.3	1.0			H2		1967LAC
		356.70	g		-1276.5	1.7	-129.2	1.7			C	c	1958SIN
		356.70	g		-1276.8	4.5	-128.9	4.5			Cl2		1956KIR
		356.70	g		-1275.3	0.8	-130.4	0.8			Cl2	c	1938CON
		356.70	l		-1236.0	2.2	-169.7	2.2	35.14	0.25	R		2019DIK
		356.70	l		-1236.4		-169.7				C		1969HU
		356.70	l		-1246.4	8.4	-159.3	8.4			C	b	1938EFT
		356.70	l		-1243.9	8.4	-161.8	8.4			C		1938EFT
		356.70	lg						35.20	0.40			2007VAR
		356.70	lg						34.40				1994CAR
		356.70	lg						35.10	0.10			1989AN
		356.70	lg						35.20	0.10			1980HUG
		356.70	lg						35.15	0.01			1968WAD
		356.70	lg						35.44	0.08			1926MAT
$C_2H_3Cl_3$	1,1,1-trichloroethane	347.22	l	SEL	-1109.1	2.0	-177.2	2.0	32.59	0.07	R		2002MAN
		347.22	g	SEL1	-1141.7	2.0	-144.6	2.0			R		2002MAN
		347.22	g		-1143.9	5.3	-142.4	5.3			R		2019DIK
		347.22	g		-1141.7	1.6	-144.6	1.6			HCl	c	1972HU
		347.22	g		-1140.31	0.84	-146.00	0.84			HCl		1972HU
		347.22	g		-1148.1	1.0	-138.2	1.0			HCl		1969HU
		347.22	l		-1111.6	5.3	-174.7	5.3	32.31	0.22	R		2019DIK
		347.22	l		-1111.8		-174.5				HCl		1975LEV
		347.22	l		-1107.73	0.80	-178.57	0.79			C		1972HU
		347.22	l		-1111.51	1.28	-174.80	1.28	32.47	0.08	C		1971MAN
		347.22	lg						32.50	0.10			1980HUG
		347.22	lg						32.47	0.06			1972LAY
	1,1,2-trichloroethane	386.78	l	SEL	-1098.0	4.0	-188.3	4.0	40.30	0.07	R		2002MAN
		386.78	g	SEL1	-1138.3	4.0	-148.0	4.0			R		2002MAN

		386.78	g		-1137.7	8.2	-148.6	8.2			R		2019DIK
		386.78	g		-1139.1	4.0	-147.2	4.0			HCl	c	1976LEV
		386.78	g		-1148.0		-138.3				C	c	1969STU
		386.78	g		-1135.4	4.5	-150.9	4.5			C	c	1956KIR
		386.78	l		-1097.5	8.2	-188.8	8.2	40.23	0.23	R		2019DIK
		386.78	l		-1097.8	4.4	-188.5	4.4			C		1987PAP
		386.78	lg						40.10	0.60			2007VAR
		386.78	lg						40.20	0.10			1980HUG
		386.78	lg						40.28	0.06			1972LAY
$C_2H_2Cl_4$	1,1,1,2-tetrachloroethane	403.33	l	SEL	-973.5	2.3	-193.4	2.3	41.10	0.50	R		2002MAN
		403.33	g	SEL1	-1014.6	2.4	-152.3	2.4			R		2002MAN
		403.33	g		-1014.14	1.13	-152.79	1.13			R		2019DIK
		403.33	g		-1191.5		24.6						1984PLA
		403.33	g		-1017.83	0.40	-149.10	0.40			HCl	c	1976LBR
		403.33	l		-973.10	1.10	-193.83	1.10			R		2019DIK
		403.33	l		-973.9	1.3	-183.5	1.4			C		1978GUN
		403.33	lg						54.80				1994SPI
		403.33	lg						47.80				1984BOU
	1,1,2,2-tetrachloroethane	419.25	l	SEL	-964.5	3.5	-202.4	3.5	45.73	0.09	R		2002MAN
		419.25	g	SEL1	-1010.2	3.5	-156.7	3.5			R		2002MAN
		419.25	g	u	-1011	8	-156	8			Cl2		1956KIR
		419.25	g		-1008.2		-158.7				CaO2	c	1956KIR
		419.25	l		-972.8	8.4	-194.1	8.4			C	b	1938EFT
		419.25	l		-971.2	8.4	-195.7	8.4			C		1938EFT
		419.25	lg						45.58	1.14	R		2019DIK
		419.25	lg						45.78	0.16			1972LAY
		419.25	lg						45.19	1.26			1926MAT
C_2HCl_5	pentachloroethane	433.45	l	SEL	-844.3	4.0	-203.3	4.0	47.40	1.50	R		2002MAN
		433.45	g	SEL1	-891.7	4.3	-155.9	4.3			R		2002MAN
		433.45	g		-892.6		-155.0				HCl	c	1979LEV
		433.45	g		-887.6		-160.0				HCl	c	1979LEV
		433.45	g		-902.4		-145.2				Cl2		1956KIR
		433.45	g		-891.8		-155.8				CaO2	b	1956KIR
		433.45	g		-891.7		-155.9				Cl2	b	1956KIR
		433.45	l		-862.3	8.4	-185.3	8.4			C	b	1938EFT
		433.45	l		-861.4	8.4	-186.2	8.4			C		1938EFT
		433.45	lg						43.9	2.4	R		2019DIK

C_2Cl_6	hexachloroethane	462.96	l	SEL	-711.7	2.8	-216.5	2.8	67.1		TN		2021RUS
		462.96	g	SEL1	-778.8	1.3	-149.4	1.3			TN		2021RUS
		462.96	g	u	-784	28	-144	28			R		2019DIK
		462.96	g	u	-780.0	5.7	-148.2	5.7			R		2002MAN
		462.96	g	u	-785	9	-143	9			D		1963PUY
		462.96	g	u	-778.9		-149.3				D	c	1963PUY
		462.96	l	u	-739	29	-189	29	45		R		2019DIK
		462.96	l	u	-729.0	6.1	-199.2	6.1	51.0	2.3	R		2002MAN
		462.96	g		-783.7		-144.5				D	c	1996HUY
		462.96	g		-781.8		-146.4				Cl2	c	1996HUY
		462.96	g		-767.5		-160.7				D	c	1979BUS
		462.96	g		-764.9		-163.3				D	c	1979BUS
		462.96	g		-777.7		-150.5				D	c	1956KIR
		462.96	g		-779.1		-149.1				D	c	1950DAI
		462.96	l		-727.4	8.4	-200.7	8.4			C		1938EFT
		462.96	sg						69.0	2.1			1974CHA
Chloroalkenes													
C_2H_3Cl	chloroethene	259.35	l	SEL	-1241.13	0.36	1.90	0.36	19.80	0.20	TN		2021RUS
		259.35	g	SEL1	-1260.93	0.30	21.70	0.30			TN		2021RUS
		259.35	g		-1261.2	3.0	22.0	3.0			R		2002MAN
		259.35	g		-1268.5	0.7	29.3	0.7			HCl		1976LEV
		259.35	g		-1261.9	0.7	22.7	0.7			HCl	c	1976LEV
		259.35	g		-1261.2	0.7	22.0	0.7			HCl	c	1976LEV
		259.35	g		-1260.2	0.7	21.0	0.7			HCl	c	1976LEV
		259.35	g		-1260.2		20.9				E		1973ALF
		259.35	g		-1274.5	1.4	35.3	1.4			HCl		1962LAC
		259.35	g		-1273.8	1.5	34.6	1.5			HCl	c	1962LAC
		259.35	g		-1262.0	2.2	22.8	2.2			C	c	1958SIN
		259.35	g		-1276.8	1.7	37.6	1.7			H2	c	1956LAC
		259.35	g		-1277.30	0.84	38.07	0.84			H2		1956LAC
		259.35	l		-1240.1	3.2	0.9	3.2	21.10	1.00	R		2002MAN
		259.35	lg						19.96	0.17	R		2019DIK
$C_2H_2Cl_2$	1,1-dichloroethene	304.71	l	SEL	-1122.81	0.49	2.95	0.49	26.75	0.15	TN		2021RUS
		304.71	g	SEL1	-1096.06	0.50	-23.80	0.50			TN		2021RUS
		304.71	g		-1121.75	0.74	1.89	0.74			R		2019DIK
		304.71	g		-1122.3	2.0	2.4	2.0			R		2002MAN
		304.71	g		-1121.4	2.1	1.5	2.1			HCl	c	1975LEV

		304.71	g		-1117.2	2.1	-2.7	2.1			HCl	c	1975LEV
		304.71	g		-1122	8	2	8			HCl	c	1972HU
		304.71	g		-1122.5	1.4	2.6	1.4			C	c	1971MAN
		304.71	g		-1122.8	1.3	2.9	1.3			C	b	1958SIN
		304.71	l		-1095.39	0.73	-24.47	0.73	26.36	0.17	R		2019DIK
		304.71	l		-1095.6	2.0	-24.3	2.0	26.74	0.09	R		2002MAN
		304.71	l		-1096.0	1.4	-24.3	1.4	26.48	0.08	C		1971MAN
		304.71	l		-1095.9		-25.1				C		1958SIN
		304.71	lg						26.48	0.08			1959HIL
	1,2-dichloroethene, (E)-	320.73	l	SEL	-1119.74	0.54	-0.12	0.54			DvH		2021RUS
		320.73	g	SEL1	-1149.24	1.14	29.38	1.14			TN		2021RUS
		320.73	g		-1119.4	2.0	-0.5	2.0			R		2002MAN
		320.73	g		-1121.5		1.7				E		1974ROZ
		320.73	g		-1119.6		-0.3				E	c	1974ROZ
		320.73	g		-1119.4		-0.5				E	c	1974ROZ
		320.73	l		-1089.9	2.2	-30.0	2.2	29.50	1.00	R		2002MAN
		320.73	l		-1095.8	8.4	-24.1	8.4			C	b	1938EFT
		320.73	l		-1094.7	8.4	-25.2	8.4			C		1938EFT
		320.73	lg						29.01	0.47	R		2019DIK
		320.73	lg	SEL					29.50	1.00	v		2002MAN
		320.73	lg						29.47				1947KET
	1,2-dichloroethene, (Z)-	333.58	l	SEL	-1086.23	1.14	-33.63	1.14			TN		2021RUS
		333.58	g	SEL1	-1117.33	0.54	-2.53	0.54			TN		2021RUS
		333.58	g		-1116.9	2.0	-3.0	2.0			R		2002MAN
		333.58	g		-1121.6	2.1	1.7	2.1			HCl	c	1975LEV
		333.58	g		-1116.3	2.1	-3.6	2.1			HCl	c	1975LEV
		333.58	g		-1124.1		4.3				E		1974ROZ
		333.58	g		-1116.7		-3.2				E	c	1974ROZ
		333.58	g		-1117.5		-2.4				E	c	1956KIR
		333.58	l		-1085.8	2.2	-34.1	2.2	31.10	1.00	R		2002MAN
		333.58	l		-1091.4		-28.5				Cl2		1956KIR
		333.58	l		-1093.7	8.4	-26.2	8.4			C	b	1938EFT
		333.58	l		-1092.3	8.4	-27.6	8.4			C		1938EFT
		333.58	lg						31.36	0.28	R		2019DIK
		333.58	lg						30.9				1947KET
C_2HCl_3	trichloroethene	360.50	l	SEL	-985.9	1.5	-14.6	1.5	34.60	0.15	TN		2021RUS
		360.50	g	SEL1	-951.3	1.5	-49.2	1.5			TN		2021RUS

		360.50	g		-981.6	4.0	-18.9	4.0			R		2019DIK
		360.50	g		-983.0	2.0	-17.5	2.0			R		2002MAN
		360.50	g		-994.6	2.9	-5.9	2.9			Cl2		1956KIR
		360.50	g		-982.0	2.9	-18.5	2.9			Cl2	c	1956KIR
		360.50	l		-947.0	4.0	-53.5	4.0	34.56	0.26	R		2019DIK
		360.50	l		-948.4	3.0	-52.1	3.0	34.57	0.09	R		2002MAN
		360.50	l		-947.7	2.9	-53.1	2.9	33.97	0.13	C		1985PAP
		360.50	l		-962.4	8.4	-1000.5	8.4			C		1938EFT
		360.50	l		-956.5	8.4	-1000.5	8.4			C	b	1938EFT
		360.50	lg										1985PAP
		360.50	lg						34.50	0.10			1980HUG
		360.50	lg						34.73	0.42			1926MAT
C_2Cl_4	tetrachloroethene	394.29	l	SEL	-818.2	1.1	-62.9	1.1	39.70	0.10	TN		2021RUS
		394.29	g	SEL1	-857.9	1.1	-23.2	1.1			TN		2021RUS
		394.29	g		-857.1	4.0	-24.0	4.0			R		2002MAN
		394.29	g		-855.2		-25.9				Cl2	c	1996HUY
		394.29	g		-853.3		-27.8				D	c	1996HUY
		394.29	g		-856.0		-25.1				HCl	c	1979LEV
		394.29	g		-861.3		-19.8				HCl	c	1979LBR
		394.29	g		-872.4		-8.7				HCl	c	1979BUS
		394.29	g		-869.4		-11.7				HCl	c	1979BUS
		394.29	g		-859.5		-21.6				HCl	c	1963PUY
		394.29	g		-858.9		-22.2				Cl2	c	1956KIR
		394.29	g		-856.8		-24.3				CaO2	b	1956KIR
		394.29	g		-857.8		-23.3				D	c	1950DAI
		394.29	g		-831.0	8.4	-50.2	8.4			C		1938EFT
		394.29	l		-817.1	4.0	-64.0	4.0	39.72	0.05	R		2002MAN
		394.29	lg						39.75	0.24	R		2019DIK
		394.29	lg						39.70	0.10			1980HUG
		394.29	lg						39.75	0.84			1926MAT
Chloroalkynes													
C_2HCl	chloroethyne	243.6	g	SEL	-1182.39	0.70	228.99	0.70			TN		2021RUS
		243.6	l	SEL1	-1162.4	1.2	209.0	1.2			DvH		2021RUS
		243.6	g			10	226	10					2002MAN
		243.6	l			10	207	10			DvH		2002MAN
		243.6	lg						32.6	1.7			2019DIK
		243.6	lg	SEL					20.0	1.0	v		2002MAN

C_2Cl_2	dichloroethyne	306.00	g		-1067.47	0.94	233.44	0.94			TN	2021RUS
		306.00	g		-1061	14	227	14			R	2002MAN
		306.00	l		-1040.1	1.5	206.0	1.5			DvH	2021RUS
		306.00	l		-1033	14	199	14			DvH	2002MAN
		306.00	lg	SEL					27.4	1.2	v	2002MAN
Bromoalkanes												
CH_3Br	bromomethane	276.70	g	SEL	-763.80	0.26	-35.61	0.26			TN	2021RUS
		276.70	l	SEL1	-740.47	0.27	-58.94	0.27			TN	2021RUS
		276.70	g		-765.1	0.8	-34.3	0.8			Br2	1973FER
		276.70	g		-761.8	1.3	-37.7	1.3			LiAl	1966ADA
		276.70	g		-761.9	1.5	-37.5	1.5			H2	1965FOW
		276.70	l		-738.8	1.3	-60.6	1.3	23.43		LiAl	1966ADA
		276.70	lg						23.09	0.27	R	2019DIK
		276.70	lg						23.91	0.30		1938EG
CH_2Br_2	dibromomethane	370.10	l	SEL	-601.3	1.1	-32.4	1.1			TN	2021RUS
		370.10	g	SEL1	-638.3	1.1	4.6	1.1			TN	2021RUS
		370.10	lg						36.91	0.32	R	2019DIK
		370.10	lg						36.97	0.10		1972LAY
$CHBr_3$	tribromomethane	422.36	l	SEL	-471.5	1.3	3.5	1.3	46.10	0.10	TN	2021RUS
		422.36	g	SEL1	-517.6	1.3	49.6	1.3			TN	2021RUS
		422.36	l		-477.4	3.3	9.4	3.3	44.42	0.53	C	1982PAP
		422.36	lg								R	2019DIK
		422.36	lg						46.05	0.10		1972LAY
CBr_4	tetrabromomethane	462.55	l	SEL	-351.6	1.4	49.3	1.4			TN	2021RUS
		462.55	g	SEL1	-406.1	1.3	103.8	1.3			TN	2021RUS
		462.55	g		-386.2	3.4	83.9	3.4			DsubH	1984BIC
		462.55	s		-331.6	1.1	29.4	1.1			R	2019DIK
		367.60	s		-331.7	3.3	29.4	3.4			C	1984BIC
		462.55	sg	SEL					54.50	0.70	s	1984BIC
		365.00	sg						54.40	0.70		1984BIC
C_2H_5Br	bromoethane	311.54	l	SEL	-1387.66	0.26	-91.05	0.26			TN	2021RUS
		311.54	g	SEL1	-1415.65	0.25	-63.06	0.25			TN	2021RUS
		311.54	g	u	-1413.4	6.3	-65.3	6.3			LiAl	1965ASH
		311.54	g		-1415.1		-63.6				R	1979KUD
		311.54	g		-1416.8	1.0	-61.9	1.0			H2	1965FOW
		311.54	g		-1414.1	2.1	-64.6	2.1			HBr	1953LAN

		311.54	l		-1383.2	2.1	-95.5	2.1			LiAl	b	1965ASH
		311.54	l		-1382.5	6.3	-96.2	6.3			LiAl		1965ASH
		311.54	lg						27.50	0.41	R		2019DIK
		311.54	lg						27.61	1.26			1953LAN
Bromoethenes													
C_2H_3Br	bromoethene	288.60	g	SEL	-1266.79	0.57	73.90	0.57			TN		2021RUS
		288.60	l	SEL1	-1233.0	1.8	40.1	1.8			DvH		2021RUS
		288.60	g		-1272.1	1.9	79.2	1.9			H2	b	1957LAC
		288.60	g		-1271.1	1.9	78.2	1.9			H2		1957LAC
		288.60	lg	SEL					33.76	1.74	v		2019DIK
Chlorofluoroalkanes													
CH_2ClF	chlorofluoromethane	264.00	g	SEL	-617.7	1.1	-263.3	1.1			TN		2021RUS
		264.00	l	SEL1	-599.1	1.5	-281.9	1.5			DvH		2021RUS
		264.00	g		-619.1	13.0	-261.9	13.0			R		1998CHA
		264.00	g		-657.0		-224.0				R		1989DAU
		264.00	lg	SEL					18.62	0.96	v		2019DIK
$CHClF_2$	chlorodifluoromethane	232.35	g	SEL	-433.99	1.01	-482.21	0.98			TN		2021RUS
		232.35	l	SEL1	-418.29	1.05	-497.91	1.03			DvH		2021RUS
		232.35	g		-433.4	2.9	-482.8	2.9			D		1965EDW
		232.35	lg	SEL					15.70	0.24	v		2019DIK
$CHCl_2F$	dichlorofluoromethane	282.05	g	SEL	-478.01	0.92	-283.59	0.91			TN		2021RUS
		282.05	l	SEL1	-454.4	1.5	-307.2	1.5			DvH		2021RUS
		282.05	g		-478.3	13.0	-283.3	13.0			R		1998CHA
		282.05	lg	SEL					23.64	1.18	v		2019DIK
$CClF_3$	chlorotrifluoromethane	191.75	g	SEL	-241.78	0.63	-709.65	0.57			TN		2021RUS
		191.75	l	SEL1	-225.28	0.70	-726.15	0.64			TN		2021RUS
		191.75	g	u	-242	28	-710	28			R		2019DIK
		191.75	g	u	-232.4	4.0	-719.0	4.0			H2		1963KOL
		191.75	g	u	-211.9	5.0	-739.5	5.0			H2	b	1963KOL
		191.75	g	u	-256	9	-695	9			D		1961BAI
		191.75	l	u	-238	28	-714	28	4.3	2.9	R		2019DIK
		191.75	g		-250.6	3.4	-700.8	3.4			I2		1967LOR
		191.75	g		-246.4	3.4	-705.0	3.4			I2	b	1967LOR
		191.75	g		-242.7	4.2	-708.8	4.2			Br2		1967COO
		191.75	g		-252.7		-698.7						1955WAR
		191.75	g		-236.0	4.2	-715.5	4.2			C		1954KIR
		191.75	lg						16.50				1987STE

CCl_2F_2	dichlorodifluoromethane	243.35	g	SEL	-303.18	0.71	-493.65	0.67			TN		2021RUS
		243.35	l	SEL1	-286.38	0.73	-510.45	0.70			DvH		2021RUS
		243.35	g	u	-327.8	5.0	-469.0	5.0			H2		1963KOL
		243.35	g	u	-319.2	5.6	-477.6	5.6			H2	b	1963KOL
		243.35	g	u	-324	13	-473	13			C		1955WAR
		243.35	g	u	-320	13	-477	13			C	b	1955WAR
		243.35	g	u	-328.2	8.4	-468.6	8.4			K		1954KIR
		243.35	l	u	-324	13	-473	13			R		2019DIK
		243.35	lg	SEL					16.80	0.23	v		2019DIK
CCl_3F	trichlorofluoromethane	296.95	g	SEL	-353.80	0.80	-288.43	0.78			TN		2021RUS
		296.95	l	SEL1	-329.01	0.81	-313.22	0.80			TN		2021RUS
		296.95	g	u	-369	27	-273	27			R		2019DIK
		296.95	g	u	-364.4	8.8	-277.8	8.8			D		1961BAI
		296.95	g	u	-373.9	8.4	-268.3	8.4			C	b	1955WAR
		296.95	g	u	-362.2	8.4	-280.0	8.4			C		1955WAR
		296.95	g	u	-349	17	-293	17			C		1954KIR
		296.95	l	u	-345	27	-298	27	24.79	0.16	R		2019DIK
C_2ClF_3	chlorotrifluoroethene	244.80	g	SEL	-833.2	2.8	-511.7	4.7			DvH		1982ERA
		244.80	l	SEL1	-816.0	2.8	-528.9	2.8	17.2	3.8	C		1982ERA
		244.80	g	u	-814	45	-531	45			R		2019DIK
		244.80	g	u	-843	13	-502	13			C		1955WAR
		244.80	g	u	-835	13	-510	13			C	b	1955WAR
		244.80	g	u	-817.7	8.4	-527.2	8.4			C		1954KIR
		244.80	l	u	-812.1	5.9	-532.8	5.9			R		2019DIK
		244.80	g		-800.1	5.4	-544.8	5.4			H2		1963KOL
		244.80	g		-780.1	5.8	-564.8	5.8			H2	b	1963KOL
		244.80	lg						17.13	0.50	R		2019DIK
Bromofluoroalkanes													
CH_2BrF	bromofluoromethane	310.00	l	SEL	-591.3	5.2	-243.4	5.2			DvH		2021RUS
		310.00	g	SEL1	-622.7	4.9	-211.9	4.9			TN		2021RUS
		310.00	lg	SEL					31.47	1.72	v		2019DIK
$CHBrF_2$	bromodifluoromethane	258.65	g	SEL	-445.5	1.2	-424.3	1.2			TN		2021RUS
		258.65	l	SEL1	-425.5	1.6	-444.4	1.5			DvH		2021RUS
		258.65	g		-444.6	0.9	-425.3	0.9			Br2		1974OKA
		258.65	lg	SEL					20.02	0.96	v		2019DIK
$CHBr_2F$	dibromofluoromethane	338.05	l	SEL	-456.9	5.2	-212.0	5.2			DvH		2021RUS

		338.05	g	SEL1	-489.6	4.9	-179.3	4.9			TN	2021RUS
		338.05	lg	SEL					32.73	1.81	v	2019DIK
$CBrF_3$	bromotrifluoromethane	215.35	g	SEL	-254.08	0.52	-651.00	0.44			TN	2021RUS
		215.35	l	SEL1	-242.31	0.53	-662.78	0.46			TN	2021RUS
		215.35	g		-255.6	3.2	-649.4	3.2			I2	1967LOR
		215.35	g		-257.7	2.9	-647.3	2.9			Br2	1967COO
		215.35	lg						11.78	0.12	R	2019DIK
CBr_2F_2	dibromodifluoromethane	297.65	g	SEL	-322.1	1.3	-382.0	1.3			TN	2021RUS
		297.65	l	SEL1	-297.7	1.3	-406.4	1.3			DvH	2021RUS
		297.65	lg	SEL					24.42	0.19	v	2019DIK
CBr_3F	tribromofluoromethane	379.65	l	SEL	-324.4	3.0	-178.9	3.0			DvH	2021RUS
		379.65	g	SEL1	-373.7	1.5	-129.5	1.5			TN	2021RUS
		379.65	lg	SEL					49.4	2.6	v	2019DIK
Bromochloroalkanes												
CH_2BrCl	bromochloromethane	341.21	l	SEL	-605.1	1.3	-74.9	1.3			DvH	2021RUS
		341.21	g	SEL1	-637.8	1.3	-42.2	1.3			TN	2021RUS
		341.21	g	u	-660	7	-20	7			Br2	1996SKO
		341.21	lg	SEL					32.75	0.18	v	2019DIK
$CHBrCl_2$	bromodichloromethane	362.65	l	SEL	-476.6	2.2	-84.1	2.2			DvH	2021RUS
		362.65	g	SEL1	-511.6	1.2	-49.1	1.2			TN	2021RUS
		362.65	lg	SEL					35.01	1.84	v	2019DIK
$CHBr_2Cl$	dibromochloromethane	393.00	l	SEL	-470.4	4.1	-44.0	4.1			DvH	2021RUS
		393.00	g	SEL1	-514.3	3.4	0.0	3.4			TN	2021RUS
		393.00	lg	SEL					44.0	2.3	v	2019DIK
$CBrCl_3$	bromotrichloromethane	376.65	l	SEL	-363.8	1.6	-77.5	1.6			DvH	2021RUS
		376.65	g	SEL1	-399.40	0.59	-41.89	0.59			TN	2021RUS
		376.65	g		-399.3	1.0	-42.0	1.0			Br2	1973MEN
		376.65	g		-402.3		-39.0				Br2	1951SUL
		376.65	lg	SEL					35.64	1.49	v	2019DIK
CBr_2Cl_2	dibromodichloromethane	423.35	l	SEL	-360.5	4.2	-34.4	4.2	-39.5		DvH	2021RUS
		423.35	g	SEL1	-400.0	1.3	5.1	1.3			TN	2021RUS
		423.35	lg	SEL					39.5	4.0	v	2019DIK
CBr_3Cl	tribromochloromethane	433.00	l	SEL	-355.0	2.9	6.4	2.9			DvH	2021RUS
		433.00	g	SEL1	-403.0	1.5	54.4	1.5			TN	2021RUS
		433.00	lg	SEL					48.1	2.5	v	2019DIK
Bromochlorofluoroalkanes												
CHBrClF	bromochlorofluoromethane	312.60	l	SEL	-456.7	5.1	-258.5	5.1	27.6		DvH	2021RUS

		312.60	g	SEL1	-484.4	4.9	-230.9	4.9			TN	2021RUS
		312.60	lg	SEL					27.62	1.52	v	2019DIK
$CBrClF_2$	bromochlorodifluoromethane	270.65	g	SEL	-310.6	4.9	-439.9	4.9			TN	2021RUS
		270.65	l	SEL1	-289.9	4.9	-460.6	4.9			DvH	2021RUS
		270.65	lg	SEL					20.72	0.12	v	2019DIK
$CBrCl_2F$	bromodichlorofluoromethane	325.15	l	SEL	-326.8	5.2	-269.1	5.2			DvH	2021RUS
		325.15	g	SEL1	-357.6	4.9	-238.3	4.9			TN	2021RUS
		325.15	lg	SEL					30.78	1.70	v	2019DIK
CBr_2ClF	dibromochlorofluoromethane	352.65	l	SEL	-327.2	5.2	-222.3	5.2			DvH	2021RUS
		352.65	g	SEL1	-362.7	4.9	-186.8	4.9			TN	2021RUS
		352.65	l	SEL					35.51	1.93	v	2019DIK
Carbonyl Halides												
CCl_2O	phosgene	280.71	g	SEL	-221.41	0.27	-219.14	0.27			TN	2021RUS
		280.71	l	SEL1	-198.58	0.47	-241.98	0.47			DvH	2021RUS
		280.71	g		-220.43	0.03	-220.12	0.04			R	2019DIK
		280.71	g		-220.43	0.96	-220.12	0.96			H2O	1972DAV
		280.71	g		-221.44	0.59	-219.12	0.59			Cl2	1970LOR
		280.71	g		-231.06	1.17	-209.49	1.17			Cl2	1969LOR
		280.71	l	SEL	-197.60	0.39	-242.96	0.39	22.84	0.39	v	2019DIK
Pentachlorophenol												
C_6HCl_5O	pentachlorophenol	463.84	s	SEL	-2329.0	2.9	-292.5	3.0			C	1958SIN
		582.50	l	SEL1	-2346.1	3.0	-275.4	3.0			DsubH	1958SIN
		582.50	g	SEL2	-2420.6	3.0	-200.9	3.0			DvH	1958SIN
		582.50	g	u	-2428	7	-194	7			R	2019DIK
		463.84	s		-2327.0	2.7	-294.4	2.7			R	2019DIK
		463.84	s		-2326.5	2.9	-295.0	3.0			C	1958SIN
		582.50	sg	SEL					91.60	0.50	s	2007VER
		463.84	sl	SEL					17.15		v	1991ACR

4.4. Recommended Heats of Combustion, Formation, and Transition

The following Table 4-4 contains the recommended values for heats of combustion $\Delta_c H$, formation $\Delta_f H$, and transition $\Delta_f H$ for many compounds, while the previous Table 4-3 contained all of the compiled values for these compounds. This table is divided into several sub-tables by primary compound class, *i.e.*, Small Molecules, Hydrocarbons, Aromatic Hydrocarbons, Oxidized Hydrocarbons, etc., and each of the sub-tables contain the compounds ordered by secondary compound class, *i.e.*, Alkanes, Alkenes, Alkadienes, Alkynes, etc., and then by molecular formula.

Table 4-4. Recommended Heats of Combustion, Formation, and Transition

Table 4-4(1). Small Molecules

Formula	Compound	T_{trs} [K]	Ph	SEL	$\Delta_c H$	u	$\Delta_f H$	u	$\Delta_{trs} H$	u	M	R	Ref
					kJ mol^{-1}								
Hydrogen/Oxygen													
H_2	hydrogen	20.37	g	SEL	-285.826	0.000	0.000	0.000			def		def
O_2	oxygen	90.19	g	SEL	0.000	0.000	0.000	0.000			def		def
H_2O_2	hydrogen peroxide	426.40	l	SEL	-98.48	0.79	-187.35	0.79	51.89	0.79	TN		2021RUS
		426.40	g	SEL1	-150.368	0.068	-135.458	0.063			TN		2021RUS
		272.74	s	SEL2	-86.26	0.79	-199.56	0.79	12.22	0.03	DfusH		1955GIG
		272.74	sl	SEL					12.22	0.03	f		1951FOL
H_2O	water	373.12	l	SEL	0.000	0.037	-285.826	0.026	44.00	0.22	TN		2021RUS
		373.12	g	SEL1	-43.994	0.037	-241.832	0.026			TN		2021RUS
		273.153	s	SEL2	6.913	0.037	-292.739	0.026	6.91		TN		2021RUS
Nitrogen/Hydrogen													
N_2	nitrogen	77.36	g	SEL	0.000	0.000	0.000	0.000			def		
H_3N	ammonia	239.82	g	SEL	-383.181	0.029	-45.558	0.029			TN		2021RUS
		239.82	l	SEL1	-363.32	0.11	-65.42	0.11			DvH		2021RUS
		239.82	lg	SEL					19.87	0.10	v		2019DIK
ClH_4NO_4	ammonium perchlorate	403.15	s(d)	SEL	-442.33	0.17	-295.77	0.17					1998CHA
H_4N_2	hydrazine	386.65	l	SEL	-622.34		50.69	0.18	-336.51	1.00			2021RUS
		386.65	g	SEL1	-669.22		97.6	1.0					2021RUS
Hydrogen Halides													
FH	hydrogen fluoride	292.7	g	SEL	na		-272.721	0.048			TN		2021RUS
		292.7	l	SEL1	na		-302.41	0.16			TN		2021RUS
	hydrogen fluoride (aq, 20 H_2O)	292.7	aq	SEL	na		-321.05	0.16			TN		2021RUS
ClH	hydrogen chloride	188.1	g	SEL	na		-92.173	0.006			TN		2021RUS
	hydrogen chloride (aq, 600 H_2O)	188.1	aq	SEL	na		-166.452	0.024			TN		2021RUS
BrH	hydrogen bromide	206.77	g	SEL	na		-36.29	0.16			R		1984COX
	hydrogen bromide (aq, 600 H_2O)	206.77	aq	SEL	na		-120.11	0.15			TN		2021RUS
Sulfur/Hydrogen/Oxygen													
H_2S	hydrogen sulfide	212.85	g	SEL	-867.21	0.5	-20.6	0.5			R		1984COX

		212.85	l	SEL1	-853.55	0.64	-34.27	0.64			DvH	1984COX
		212.85	lg	SEL					13.67	0.40	v	2019DIK
O_2S	sulfur dioxide	263.14	l	SEL	na		-320.5	1.0	23.67		R	1982WAG
		263.14	g	SEL1	na		-296.83	0.20			R	1982WAG
H_2O_4S	sulfuric acid	283.46	l	SEL1	na		-814.0	1.0			R	1982WAG
		283.46	g	SEL2	na		-735.1	1.0			R	1998CHA
	sulfuric acid (aq, 115 H_2O)	283.46	aq	SEL	na		-887.81	0.25			R	1982WAG
Boron Compounds												
BH_3O_3	boric acid	444.05	s	SEL	na		-1091.94	0.13			D	1950SMI
	boric acid (aq, 500 H_2O)	444.05	aq	SEL	na		-1069.89	0.13			H2O	1950SMI
B_2H_6	diborane	180.59	g	SEL	-2175.76	1.17	36.0	1.2			D	1965GUN
		180.59	l	SEL1	-2174.75	1.17	35.0	1.2			DvH	1965GUN
		180.59	lg	SEL			36.8		1.01		v	1959PAR
B_2O_3	diboron trioxide	723.15	s	SEL	na		-1279.9	2.1				1959JOH
		2130	g	SEL1	na		-836.0	4.2				1963HIL
		2130	l	SEL2	na		-1259.3	1.3				1961NBS

Table 4-4(2). Hydrocarbons

Formula	Compound	T_{trs} [K]	Ph	SEL	$\Delta_c H$ kJ mol^{-1}	*u*	$\Delta_f H$	*u*	$\Delta_{trs} H$	*u*	M	R	Ref
Carbon													
C	diamond	4300	s	SEL1	-395.347	0.070	1.871	0.070			C		1966HAW
	graphite	4800	s	SEL	-393.476	0.025	0.000	0.025			def		1966HAW
		5000	g	SEL1	-1110.359	0.047	716.883	0.045			TN		2021RUS
Alkanes													
CH_4	methane	111.67	g	SEL	-890.602	0.050	-74.526	0.049			TN		2021RUS
C_2H_6	ethane	184.57	g	SEL	-1560.39	0.13	-84.04	0.13			TN		2021RUS
		184.57	l	SEL1	-1555.58	1.03	-88.85	1.03			DvH		2021RUS
		184.57	g	SEL	-1560.34	0.99	-84.09	0.99	4.81	0.29	v		2019DIK
C_3H_8	propane	231.04	g	SEL	-2218.66	0.16	-105.07	0.16			TN		2021RUS
		231.04	l	SEL1	-2203.31	0.26	-120.42	0.26			DvH		2021RUS
		231.04	lg	SEL					15.4		v		1945PRO
C_4H_{10}	isobutane	261.40	g	SEL	-2868.41	0.30	-134.62	0.30			TN		2021RUS
		261.40	l	SEL1	-2848.95	0.37	-154.08	0.37			DvH		2021RUS
		261.40	l	SEL	-2848.6	1.7	-154.4	1.7	19.46	0.21	v		2019DIK
	n-butane	272.66	g	SEL	-2877.28	0.24	-125.75	0.24			TN		2021RUS
		272.66	l	SEL1	-2854.88	0.69	-148.15	0.69			DvH		2021RUS
		272.66	lg	SEL					22.40		v		1971WIL
C_5H_{12}	isopentane	300.98	l	SEL	-3503.95	0.43	-178.39	0.43			TN		2021RUS
		300.98	g	SEL1	-3529.17	0.43	-153.17	0.43			TN		2021RUS
		300.98	lg	SEL					25.22		v		1985MAJ
	neopentane	282.65	l	SEL	-3492.56	0.39	-189.78	0.39	22.39	0.30	TN		2021RUS
		282.65	g	SEL1	-3514.95	0.39	-167.39	0.39			TN		2021RUS
	n-pentane	309.21	l	SEL	-3509.35	0.43	-172.99	0.43	26.74	0.20	TN		2021RUS
		309.21	g	SEL1	-3536.09	0.31	-146.25	0.31			TN		2021RUS
C_6H_{14}	3-methylpentane	336.43	l	SEL	-4159.90	0.88	-201.74	0.96	30.30	0.10	C		1945PRO
		336.43	g	SEL1	-4190.2	1.0	-171.4	1.0			DvH		1945PRO
		336.43	lg	SEL					30.27	0.10	v		1947OSB
	isohexane	333.42	l	SEL	-4157.65	0.83	-203.99	0.83	30.11	0.20	TN		2021RUS
		333.42	g	SEL1	-4187.76	0.84	-173.88	0.84			TN		2021RUS
	neohexane	322.89	l	SEL	-4148.50	0.88	-213.14	0.96	27.68	0.20	C		1945PRO
		322.89	g	SEL1	-4176.18	0.96	-185.46	0.96			DvH		1945PRO
		322.89	lg	SEL					27.68		v		1947OSB

	n-hexane	341.87	l	SEL	-4163.04	0.34	-198.60	0.34	31.71	0.20	TN	2021RUS
		341.87	g	SEL1	-4194.75	0.39	-166.89	0.39			TN	2021RUS
C_7H_{16}	n-heptane	371.55	l	SEL	-4816.83	0.46	-224.11	0.46	36.65	0.20	TN	2021RUS
		371.55	g	SEL1	-4853.48	0.46	-187.46	0.46			TN	2021RUS
C_8H_{18}	n-octane	398.79	l	SEL	-5470.63	0.55	-249.61	0.55	41.53	0.20	TN	2021RUS
		398.79	g	SEL1	-5512.16	0.54	-208.08	0.54			TN	2021RUS
C_9H_{20}	n-nonane	423.91	l	SEL	-6124.85	0.50	-274.69	0.50	46.44	0.20	TN	2021RUS
		423.91	g	SEL1	-6171.29	0.51	-228.25	0.51			TN	2021RUS
$C_{10}H_{22}$	n-decane	447.27	l	SEL	-6778.29	0.80	-300.56	0.80	51.39	0.20	TN	2021RUS
		447.27	g	SEL1	-6829.68	0.91	-249.17	0.91			TN	2021RUS
$C_{16}H_{34}$	n-hexadecane	559.94	l	SEL	-10699.1	1.8	-455.6	2.0	81.40	0.40	C	1955FRA
		559.94	g	SEL1	-10780.5	1.8	-374.2	2.0			DvH	1955FRA
		559.94	lg	SEL					81.4		v	1995CHI
Alkenes												
C_2H_4	ethene	169.38	g	SEL	-1410.92	0.12	52.32	0.12			TN	2021RUS
		169.38	l	SEL1	-1402.48	0.17	43.88	0.17			DvH	2021RUS
		169.38	l	SEL	-1402.7	2.7	44.1	2.7	8.44	0.13	v	2019DIK
C_3H_6	propene	225.53	g	SEL	-2057.79	0.20	19.88	0.19			TN	2021RUS
		225.53	l	SEL1	-2043.57	0.33	5.66	0.33			DvH	2021RUS
		225.53	l	SEL	-2042.3	2.5	4.4	2.5	14.22	0.27	v	2019DIK
C_4H_8	1-butene	266.83	g	SEL	-2717.30	0.36	0.09	0.36			TN	2021RUS
		266.83	l	SEL1	-2697.20	0.45	-20.01	0.45			DvH	2021RUS
		266.83	lg	SEL					20.1		v	1971WIL
	2-butene, (E)-	274.01	g	SEL	-2706.07	0.38	-11.14	0.38			TN	2021RUS
		274.01	l	SEL1	-2684.77	0.41	-32.44	0.41			DvH	2021RUS
		274.01	lg	SEL					21.3		v	1971WIL
	2-butene, (Z)-	276.87	g	SEL	-2710.16	0.40	-7.05	0.40			TN	2021RUS
		276.87	l	SEL1	-2688.06	0.59	-29.15	0.59			DvH	2021RUS
		276.87	lg	SEL					22.1		v	1971WIL
	isobutene	266.05	g	SEL	-2700.20	0.39	-17.01	0.39			TN	2021RUS
		266.05	l	SEL1	-2679.60	0.50	-37.61	0.49			DvH	2021RUS
		266.05	lg	SEL					20.60		v	1971WIL
C_5H_8	2-methyl-1,3-butadiene	307.19	l	SEL	-3159.50	0.72	48.82	0.72			DvH	2021RUS
		307.19	g	SEL1	-3186.28	0.67	75.60	0.67			TN	2021RUS
		307.19	lg	SEL					26.78	0.25	v	1971ROG
C_5H_{10}	1-pentene	303.12	l	SEL	-3349.72	0.64	-46.79	0.64			C	1979GOO
		303.12	g	SEL1	-3375.22	0.67	-21.29	0.67			DvH	1979GOO

		303.12	lg	SEL					25.5		v	1971WIL
	2-methyl-1-butene	304.30	l	SEL	-3335.74	0.84	-60.77	0.84			C	1979GOO
		304.30	g	SEL1	-3361.64	0.86	-34.87	0.86			DvH	1979GOO
		304.30	lg	SEL					25.9		v	1971WIL
	2-pentene, (E)-	309.51	l	SEL	-3338.71	0.76	-57.80	0.76			C	1979GOO
		309.51	g	SEL1	-3365.4	0.8	-31.1	0.8			DvH	1979GOO
		309.51	lg	SEL					26.7		v	1971WIL
	2-pentene, (Z)-	310.09	l	SEL	-3343.21	0.62	-53.30	0.62			C	1979GOO
		310.09	g	SEL1	-3370.0	0.7	-26.5	0.7			DvH	1979GOO
		310.09	lg	SEL					26.8		v	1971WIL
	3-methyl-1-butene	293.21	g	SEL	-3369.00	0.68	-27.51	0.68			DvH	1979GOO
		293.21	l	SEL1	-3345.10	0.62	-51.41	0.62			C	1979GOO
		293.21	lg	SEL					23.9		v	1971WIL
C_6H_{12}	1-hexene	336.64	l	SEL	-4003.1	1.2	-72.7	1.2			H2	1984MOL
		336.64	g	SEL1	-4033.7	1.2	-42.1	1.2			DvH	1984MOL
		336.64	lg	SEL					30.60		v	1971WIL
C_7H_{14}	1-heptene	366.71	l	SEL	-4657.41	0.63	-97.70	0.63			H2O	1984WIB
		366.71	g	SEL1	-4693.1	0.7	-62.0	0.7			DvH	1984WIB
		366.71	lg	SEL					35.7		v	1971WIL
C_8H_{16}	1-octene	394.43	l	SEL	-5312.9	1.2	-121.5	1.2			C	1961ROC
		394.43	g	SEL1	-5353.5	1.2	-80.9	1.2			DvH	1961ROC
		394.43	lg	SEL					40.60		v	1995CHI
Alkadienes												
C_3H_4	allene	238.65	g	SEL	-1941.86	0.24	189.78	0.24			TN	2021RUS
		238.65	l	SEL1	-1925.30	0.69	173.22	0.69			DvH	2021RUS
		238.65	l	SEL	-1931.3	4.8	179.3	4.8	16.56	0.65	v	2019DIK
C_4H_6	1,2-butadiene	284.06	g	SEL	-2593.79	0.46	162.41	0.46	23.68	0.30	TN	2021RUS
		284.06	l	SEL1	-2570.11	0.66	138.73	0.66			TN	2021RUS
	1,3-butadiene	268.44	g	SEL	-2542.28	0.33	110.90	0.33			TN	2021RUS
		268.44	l	SEL1	-2521.18	0.43	89.80	0.43			DvH	2021RUS
		268.44	lg	SEL					21.1		v	1971WIL
C_5H_8	1,2-pentadiene	318.80	l	SEL	-3222.90	0.69	112.22	0.69			DvH	1955FRA
		318.80	g	SEL1	-3251.60	0.67	140.92	0.67			C	1955FRA
		318.80	lg	SEL					28.7		v	1971WIL
	1,3-pentadiene, (E)-	315.32	l	SEL	-3158.90	0.78	48.22	0.78			DvH	1955FRA
		315.32	g	SEL1	-3186.70	0.67	76.02	0.67			C	1955FRA
		315.32	lg	SEL					27.8		v	1971WIL

	1,3-pentadiene, (Z)-	317.18	l	SEL	-3165.3	1.4	54.6	1.4			DvH	1955FRA
		317.18	g	SEL1	-3193.60	0.92	82.92	0.92			C	1955FRA
		317.18	lg	SEL					28.30	0.40	v	1971WIL
	1,4-pentadiene	299.12	g	SEL	-3217.2	1.3	106.5	1.3			C	1955FRA
		299.12	l	SEL1	-3192.0	1.3	81.3	1.3	25.20	0.20	DvH	1955FRA
		299.12	lg	SEL					25.2		v	1971WIL
Alkynes												
C_2H_2	acetylene	188.41	g	SEL	-1301.06	0.13	228.28	0.13			TN	2021RUS
		188.41	l	SEL1	-1293.7	4.4	220.9	4.4			DvH	2021RUS
		188.41	l	SEL	-1291.8	4.7	219.0	4.7	7.4	4.4	v	2019DIK
C_3H_4	propyne	249.80	g	SEL	-1937.72	0.22	185.64	0.22			TN	2021RUS
		249.80	l	SEL1	-1918.14	0.56	166.06	0.56			DvH	2021RUS
		249.80	l	SEL	-1918.5	3.8	166.5	3.8	19.58	0.51	v	2019DIK
C_4H_6	1-butyne	281.18	g	SEL	-2598.06	0.67	166.68	0.67			TN	2021RUS
		281.18	l	SEL1	-2574.36	0.71	142.98	0.71			DvH	2021RUS
		281.18	lg	SEL					23.7		v	1971WIL
	2-butyne	300.12	l	SEL	-2551.15	0.58	119.77	0.57			DvH	2021RUS
		300.12	g	SEL1	-2577.85	0.49	146.47	0.49			TN	2021RUS
		300.12	lg	SEL					26.7		v	1971WIL
C_5H_8	1-pentyne	313.51	l	SEL	-3226.6	2.3	115.9	2.3			DvH	1945WAG
		313.51	g	SEL1	-3255.0	2.1	144.3	2.1			E	1945WAG
		313.51	lg	SEL					28.4		v	1971WIL
	2-pentyne	329.27	l	SEL	-3208.8	2.2	98.1	2.2			DvH	1945WAG
		329.27	g	SEL1	-3239.6	2.1	128.9	2.1			E	1945WAG
		329.27	lg	SEL					30.8		v	1971WIL
C_6H_{10}	1-hexyne	344.53	l	SEL	-3879.3	1.6	89.4	1.6			DvH	1979ROG
		344.53	g	SEL1	-3912.3	1.2	122.3	1.2			H2	1979ROG
		344.53	l	SEL	-3881.3	2.1	91.4	2.1	32.94	0.29	v	2019DIK
	2-hexyne	357.59	l	SEL	-3861.9	2.5	71.9	2.5			DvH	1979ROG
		357.59	g	SEL1	-3897.7	2.4	107.7	2.4			H2	1979ROG
		357.59	lg	SEL					35.8		v	2007BOU
	3-hexyne	354.58	l	SEL	-3860.2	1.9	70.2	1.9			DvH	1979ROG
		354.58	g	SEL1	-3895.4	1.9	105.4	1.9			H2	1979ROG
		354.58	l	SEL	-3864.8	2.6	74.9	2.6	35.21	0.29	v	2019DIK
C_4H_4	butenyne	279.18	g	SEL	-2434.97	0.58	289.41	0.58			TN	2021RUS
		279.18	l	SEL1	-2411.8	2.1	266.2	2.1	23.21	0.40	TN	2021RUS
C_5H_6	3-penten-1-yne	317.05	l	SEL	-3050.7	3.6	225.9	3.6	27.58	1.50	R	2019DIK

		317.05	g	SEL1	-3078.3	3.3	253.4	3.3			R	2019DIK
	3-penten-1-yne, (E)-	323.65	l	SEL	-3050.7	3.2	225.9	3.2	28.35	1.54	R	2019DIK
		323.65	g	SEL1	-3079.1	2.8	254.2	2.8			R	2019DIK
	3-penten-1-yne, (Z)-	317.15	l	SEL	-3050.2	2.9	225.4	2.9	27.28	0.77	R	2019DIK
		317.15	g	SEL1	-3077.5	2.8	252.6	2.8			R	2019DIK
C_4H_2	butadiyne	283.65	g	SEL	-2319.73	0.58	460.00	0.58			TN	2021RUS
		283.65	l	SEL1	-2296.49	1.17	436.76	1.16			DvH	2021RUS
		283.65	l	SEL	-2297.1	3.1	437.4	3.1	23.24	1.01	v	2019DIK
Cycloalkanes												
C_3H_6	cyclopropane	240.27	g	SEL	-2091.75	0.40	53.84	0.40			TN	2021RUS
		240.27	l	SEL1	-2073.63	0.53	35.72	0.53	18.12	0.20	TN	2021RUS
C_4H_8	cyclobutane	285.64	g	SEL	-2745.02	0.39	27.81	0.39			TN	2021RUS
		285.64	l	SEL1	-2721.14	0.40	3.93	0.40	23.88	0.30	TN	2021RUS
C_5H_{10}	cyclopentane	322.40	l	SEL	-3291.40	0.43	-105.11	0.42	28.69	0.20	TN	2021RUS
		322.40	g	SEL1	-3320.09	0.43	-76.42	0.42			TN	2021RUS
	methylcyclobutane	310.00	l	SEL	-3339.5	1.3	-57.1	1.3			DvH	1950HUM
		310.00	g	SEL1	-3352.0	1.3	-44.5	1.3			C	1950HUM
		310.00	l	SEL	-3365.4	2.9	-31.1	2.9	25.92	1.30	v	2019DIK
C_6H_{12}	cyclohexane	353.87	l	SEL	-3919.73	0.30	-156.08	0.29	33.14	0.15	TN	2021RUS
		353.87	g	SEL1	-3952.87	0.31	-122.94	0.30			TN	2021RUS
	methylcyclopentane	344.96	l	SEL	-3937.74	0.37	-138.07	0.36	31.78	0.15	TN	2021RUS
		344.96	g	SEL1	-3969.52	0.38	-106.29	0.37			TN	2021RUS
C_7H_{14}	methylcyclohexane	374.12	l	SEL	-4565.29	0.96	-189.82	1.05	35.40	0.20	C	1946PRO
		374.12	g	SEL1	-4600.69	1.08	-154.42	1.08			DvH	1946PRO
$C_{10}H_{20}$	1,3-diethylcyclohexane	445.70	l	SELu	-6515.9	6.2	-277.1	6.2	46.83	1.55	R	2019DIK
		445.70	g	SEL1u	-6562.7	6.0	-230.3	6.0			R	2019DIK
Cycloalkenes												
C_4H_6	cyclobutene	275.74	g	SEL	-2591.98	0.71	160.60	0.71			TN	2021RUS
		275.74	l	SEL1	-2569.73	0.74	138.35	0.74			DvH	2021RUS
		275.74	l	SEL	-2565.8	1.7	134.4	1.7	22.26	0.21	v	2019DIK
C_5H_8	cyclopentene	317.39	l	SEL	-3117.56	0.52	6.88	0.52	28.29	0.30	TN	2021RUS
		317.39	g	SEL1	-3145.85	0.47	35.17	0.47			TN	2021RUS
	methylenecyclobutane	315.00	l	SEL	-3204.7	0.5	94.0	0.5	27.70	0.42	C	1974GOO
		315.00	g	SEL1	-3232.40	0.65	121.72	0.65			C	1974GOO
C_6H_{10}	cyclohexene	356.10	l	SEL	-3752.00	0.32	-37.99	0.31	33.56	0.53	TN	2021RUS
		356.10	g	SEL1	-3785.56	0.33	-4.43	0.32			TN	2021RUS
Bicycloalkanes												

$C_{10}H_{12}$	tetralin	480.56	l	SEL	-5621.5	1.0	-28.2	1.0			C	1976GOO
		480.56	g	SEL1	-5676.5	1.4	26.8	1.4			DvH	1976GOO
		480.56	lg	SEL					55.00	1.00	v	1971BOY
$C_{10}H_{18}$	cis-decalin	468.93	l	SEL	-6287.7	1.3	-219.5	1.3	50.2	2.1	C	1941DAV
		468.93	g	SEL1	-6337.9	2.5	-169.3	2.5			DvH	1941DAV
		468.93	lg	SEL					50.2	2.1	v	1960SPE
	trans-decalin	460.42	l	SEL	-6278.9	1.3	-228.3	1.3			C	1941DAV
		460.42	g	SEL1	-6327.4		-179.8				DvH	1941DAV
		460.42	lg	SEL					48.5	2.1	v	1960SPE
$C_{12}H_{22}$	1,1'-bicyclohexyl	511.10	l	SEL	-7593.0	1.2	-272.8	1.2			C	1976GOO
		511.10	g	SEL1	-7651.0	0.3	-214.8	1.2			DvH	1976GOO
		511.10	lg	SEL					57.98		v	1985MAJ
$C_{10}H_{12}$	tetralin	480.56	l	SEL	-5621.5	0.9	-28.2	1.0			C	1976GOO
		480.56	g	SEL1	-5676.54	1.05	26.82	1.04			DvH	1976GOO
		480.56	lg	SEL					55.00	0.30	v	1971BOY

Table 4-4(3). Aromatic Hydrocarbons

Formula	Compound	T_{trs} [K]	Ph	SEL	$\Delta_c H$	*u*	$\Delta_f H$ kJ mol^{-1}	*u*	$\Delta_{trs} H$	*u*	M	R	Ref
C_6H_6	benzene	353.22	l	SEL	-3267.51	0.23	49.18	0.22	33.94	0.15	TN		2021RUS
		353.22	g	SEL1	-3301.45	0.23	83.12	0.22			TN		2021RUS
		278.70	s	SEL2	-3256.83	0.92	38.50	0.92	10.50	0.20	DfusH		2008ROU
		278.70	sl	SEL					10.50	0.20	f		2008ROU
C_7H_8	toluene	383.75	l	SEL	-3909.71	0.34	12.07	0.33	38.04	0.25	TN		2021RUS
		383.75	g	SEL1	-3947.7		50.1				TN		2021RUS
		178.20	s	SEL2	-3899.8	1.5	2.1	1.5	9.90	1.10	R		2008ROU
C_8H_{10}	ethylbenzene	408.96	l	SEL	-4564.41	0.55	-12.53	0.55	42.26	0.40	TN		2021RUS
		408.96	g	SEL1	-4606.67	0.55	29.73	0.55			TN		2021RUS
	m-xylene	412.25	l	SEL	-4551.86	0.63	-25.08	0.63	42.60	0.30	C		1946PRO
		412.25	g	SEL1	-4594.46	0.69	17.52	0.69			DvH		1946PRO
	o-xylene	417.56	l	SEL	-4552.9	1.0	-24.1	1.0	43.40	0.30	C		1945PRO
		417.56	g	SEL1	-4596.26	1.04	19.32	1.04			DvH		1945PRO
	p-xylene	411.47	l	SEL	-4552.86	0.92	-24.08	0.92	42.30	0.30	C		1946PRO
		411.47	g	SEL1	-4595.16	0.97	18.22	0.97			C(l)		1946PRO
C_9H_{12}	isopropylbenzene	425.54	l	SEL	-5215.44	0.96	-40.80	0.97			C		1945PRO
		425.54	g	SEL1	-5260.54	1.09	4.30	1.09			DvH		1945PRO
		425.54	lg	SEL					45.14		v		1947OSB
$C_{10}H_{14}$	m-isopropyltoluene	448.35	l	SEL	-5857.3	1.0	-78.2	1.0			C		1973GOO
		448.35	g	SEL1	-5906.9	1.3	-28.7	1.3			DvH		1973GOO
		448.35	l	SEL	-5856.3	1.7	-79.2	1.7	49.55	0.88	v		2019DIK
	o-isopropyltoluene	451.50	l	SEL	-5862.62	0.84	-72.92	0.84			C		1973GOO
		451.50	g	SEL1	-5912.26	1.19	-23.28	1.19			DvH		1973GOO
		451.50	l	SEL	-5861.7	1.6	-73.9	1.6	49.64	0.84	v		2019DIK
	p-isopropyltoluene	450.27	l	SEL	-5857.9	1.0	-77.6	1.0			C		1973GOO
		450.27	g	SEL1	-5907.28	1.11	-28.26	1.10			DvH		1973GOO
		450.27	l	SEL	-5856.9	1.6	-78.7	1.6	49.39	0.47	v		2019DIK
C_8H_8	styrene	418.45	l	SEL	-4395.42	0.48	104.31	0.48	44.03	0.40	TN		2021RUS

		418.45	g	SEL1	-4439.45	0.48	148.34	0.48			TN	2021RUS
$C_{10}H_8$	naphthalene	353.65	s	SEL	-5154.7	3.4	78.0	1.5	16.90	0.70	R	2008ROU
		353.65	l	SEL1	-5173.0	1.7	94.9	1.7			DvH	2008ROU
		491.11	g	SEL2	-5228.7	1.5	150.6	1.5			R	2008ROU
		491.11	lg	SEL					55.40	1.40	v	2008ROU
		353.65	sl	SEL					16.90	0.70	f	2008ROU
$C_{11}H_{10}$	1-methylnaphthalene	517.84	l	SEL	-5814.0	1.7	56.7	1.7	60.10	0.80	C	1960SPE
		517.84	g	SEL1	-5874.1	1.9	116.8	1.9			DvH	1960SPE
		242.52	s	SEL2	-5807.1	1.7	49.7	1.7			DfusH	1960SPE
		517.84	lg	SEL					60.10	0.80	v	2003VER
		242.52	sl	SEL					6.95	1.00	f	1996DOM
	2-methylnaphthalene	307.69	s	SEL	-5802.7	1.5	45.3	1.5	12.13	1.00	C	1960SPE
		514.25	l	SEL1	-5814.8	2.2	57.5	2.4			DfusH	1960SPE
		514.25	g	SEL2	-5860.1	1.8	102.8	2.6			DvH	1960SPE
		514.25	lg	SEL					45.31	1.00	v	1957GLA
		307.69	sl	SEL					12.13	1.00	f	1996DOM
C_8H_8	styrene	418.45	l	SEL	-4394.87	0.84	103.76	0.84	43.50	0.40	C	1945PRO
		418.45	g	SEL1	-4438.35	0.92	147.24	0.92			C	1945PRO

Table 4-4(4). Oxidized Hydrocarbons

Formula	Compound	T_{trs} [K]	Ph	SEL	$\Delta_c H$	*u*	$\Delta_f H$ kJ mol^{-1}	*u*	$\Delta_{trs} H$	*u*	M	R	Ref
Carbon Oxides													
CO_2	carbon dioxide	194.69	g	SEL	0.000	0.021	-393.476	0.015			TN		2021RUS
CO	carbon monoxide	81.64	g	SEL	-282.952	0.030	-110.524	0.026			TN		2021RUS
Alkanols													
CH_4O	methanol	337.63	l	SEL	-726.52	0.16	-238.61	0.15	37.70	0.05	TN		2021RUS
		337.63	g	SEL1	-764.22	0.16	-200.91	0.15			TN		2021RUS
C_2H_6O	ethanol	351.57	l	SEL	-1366.92	0.23	-277.51	0.22	42.47		TN		2021RUS
		351.57	g	SEL1	-1409.39	0.23	-235.04	0.22			TN		2021RUS
C_3H_8O	1-propanol	370.26	l	SEL	-2021.03	0.25	-302.70	0.24	47.46		TN		2021RUS
		370.26	g	SEL1	-2068.49	0.26	-255.24	0.25			TN		2021RUS
	isopropanol	355.39	l	SEL	-2004.83	0.36	-318.90	0.36	45.44	0.10	TN		2021RUS
		355.39	g	SEL1	-2050.27	0.36	-273.46	0.36			TN		2021RUS
$C_4H_{10}O$	1-butanol	390.77	l	SEL	-2676.18	0.24	-326.85	0.25			C		1975MOS
		390.77	g	SEL1	-2728.68	0.39	-274.35	0.38			DvH		1975MOS
		390.77	lg	SEL					52.50		v		1995CHI
	isobutanol	380.90	l	SEL	-2669.64	0.59	-333.39	0.59			C		1965CHA
		380.90	g	SEL1	-2720.48	0.59	-282.56	0.59			DvH		1965CHA
		380.90	lg	SEL					50.84	0.08	v		1966WAD
	tert-butanol	355.50	l	SEL	-2643.95	0.79	-359.08	0.80	46.30		C		1960SKI
		355.50	g	SEL1	-2689.7	1.5	-313.4	1.5			DvH		1960SKI
		298.87	s	SEL2	-2636.7	5.1	-366.4	5.1	7.24		R		2019DIK
$C_5H_{12}O$	1-pentanol	410.90	l	SEL	-3330.91	0.28	-351.43	0.29			C		1975MOS
		410.90	g	SEL1	-3387.60	0.35	-294.74	0.34			DvH		1975MOS
		410.90	lg	SEL					56.69		v		1965CHA
	2-methyl-1-butanol	402.14	l	SEL	-3325.95	0.54	-356.39	0.55	54.56	1.26	C		1965CHA
	isopentanol	404.73	l	SEL	-3326.2	0.5	-356.1	0.5	55.02	1.26	C		1965CHA
		404.73	g	SEL1	-3381.2	1.4	-301.1	1.4			DvH		1965CHA

Sugars												
$C_2H_6O_2$	1,2-ethanediol	470.73	l	SEL	-1189.19	0.37	-455.24	0.37	65.87	0.20	TN	2021RUS
		470.73	g	SEL1	-1255.06	0.40	-389.37	0.40			TN	2021RUS
$C_3H_8O_2$	2-methoxyethanol	397.54	l	SEL	-1901.7	7.6	-422.0	7.6	45.1	2.7	H2O	1977GUT
		397.54	g	SEL1	-1947	8	-377	8			DvH	1977GUT
$C_3H_8O_3$	glycerin	563.00	l	SEL	-1654.3	0.4	-669.4	0.4	91.70	0.90	C	1988BAS
		563.00	g	SEL1	-1746.00	0.99	-577.73	0.98			DvH	1988BAS
		563.00	s	SEL2	-1636.02	0.99	-687.71	0.98			DfusH	1988BAS
		563.00	lg	SEL					85.77		v	1962ROS
		291.05	sl	SEL					18.28		f	1991ACR
$C_6H_{12}O_6$	alpha-D-glucose	415.0	s	SEL	-2805.0	1.3	-1270.8	1.3			C	1960PON
		706	g	SEL1	-2944	49	-1132	49			DsubH	1960PON
		415.0	sg	SEL					139	49	s	2019DIK
$C_6H_{12}O_6$	fructose	415.0	s(d)	SEL	-2810.4	0.3	-1265.4	0.3			C	1939CLA
$C_{12}H_{22}O_{11}$	sucrose	415.0	s(d)	SEL	-5643.4	1.8	-2222.4	1.8			C	1960PON
Ethers												
C_2H_6O	dimethyl ether	248.37	g	SEL	-1460.41	0.40	-184.02	0.40			TN	2021RUS
		248.37	l	SEL1	-1441.9	1.1	-202.5	1.1			DvH	2021RUS
		248.37	lg	SEL					18.50		v	1976AMB
C_3H_8O	ethyl methyl ether	280.59	g	SEL	-2106.41	0.58	-217.32	0.58			DvH	2021RUS
		280.59	l	SEL1	-2082.5	1.2	-241.2	1.2			TN	2021RUS
		280.59	l	SEL	-2083.4	1.9	-240.3	1.9	23.90	1.10	v	2019DIK
$C_4H_{10}O$	diethyl ether	307.56	l	SEL	-2725.25	0.82	-277.78	0.82	27.37	0.25	TN	2021RUS
		307.56	g	SEL1	-2752.62	0.82	-250.41	0.82			TN	2021RUS
$C_6H_{14}O$	diisopropyl ether	341.49	l	SEL	-4010.4	1.3	-351.2	1.3			C	1965COL
		341.49	g	SEL1	-4043.1	1.4	-318.5	1.4			DvH	1965COL
		341.49	lg	SEL					32.70	0.50	v	2007EFI
Aldehydes												
CH_2O	formaldehyde	254.13	g	SEL	-570.088	0.096	-109.214	0.096			TN	2021RUS
		254.13	l	SEL1	-549.65	0.55	-129.65	0.55	20.44	0.54	TN	2021RUS
C_2H_4O	acetaldehyde	293.56	g	SEL	-1193.06	0.25	-165.54	0.25			TN	2021RUS
		293.56	l	SEL1	-1166.84	0.47	-191.76	0.47	26.22	0.40	TN	2021RUS

C_3H_6O	propanal	321.19	l	SEL	-1821.20	0.36	-216.71	0.35	29.94	0.25	TN	2021RUS
		321.19	g	SEL1	-1851.14	0.26	-186.77	0.25			TN	2021RUS
C_4H_8O	butanal	347.95	l	SEL	-2477.72	0.84	-239.49	0.84	33.68	0.42	TN	2021RUS
		347.95	g	SEL1	-2511.40	0.85	-205.81	0.85			TN	2021RUS
C_3H_4O	1-propenal	264.25	g	SEL	-1687.9		-64.2	1.1			TN	2021RUS
	2-propenal	325.40	l	SEL	-1656.4	1.4	-95.7	1.4	30.00	0.30	TN	2021RUS
		325.40	g	SEL1	-1686.4	1.2	-65.7	1.2			TN	2021RUS
Ketones												
C_3H_6O	acetone	329.22	l	SEL	-1789.79	0.35	-248.12	0.35	31.38	0.10	TN	2021RUS
		329.22	g	SEL1	-1821.17	0.35	-216.74	0.35			TN	2021RUS
C_4H_8O	butanone	352.74	l	SEL	-2443.83	0.79	-273.38	0.79	34.92	0.10	TN	2021RUS
		352.74	g	SEL1	-2478.75	0.79	-238.46	0.79			TN	2021RUS
Carboxylic Acids												
CH_2O_2	formic acid	374.05	l	SEL	-254.59	0.20	-424.71	0.20	46.33		TN	2021RUS
		374.05	g	SEL1	-300.92	0.22	-378.38	0.22			TN	2021RUS
		281.47	s	SEL2	-241.9	1.0	-437.4	1.0	12.68	1.00	DfusH	2021RUS
		281.47	sl	SEL					12.68	1.00	f	1941STO
$C_2H_4O_2$	acetic acid	391.20	l	SEL	-874.95	0.18	-483.65	0.18	50.91	0.30	TN	2021RUS
		391.20	g	SEL1	-925.86	0.38	-432.74	0.38			TN	2021RUS
		289.70	s	SEL2	-863.23	0.35	-495.37	0.35			DfusH	2021RUS
		289.70	sl	SEL					11.72		f	1996DOM
C_3H_6O	propanoic acid	413.99	l	SEL	509.60	0.18	-509.60	0.18	55.36	0.20	TN	2021RUS
		413.99	g	SEL1	454.24	0.28	-454.24	0.28			TN	2021RUS
C_4H_8O	n-butanoic acid	436.42	l	SEL	-2183.50	0.59	-533.70	0.59			C	1964LEB
		436.42	g	SEL1	-2241.73	0.43	-475.47	0.42			DvH	1964LEB
		436.42	lg	SEL					58.23	0.30	v	2000VER
Esters												
$C_3H_6O_2$	ethyl formate	327.29	l	SEL	-1611.8	1.2	-426.1	1.2	32.10	0.15	TN	2021RUS
		327.29	g	SEL1	-1643.9	1.2	-394.0	1.2			TN	2021RUS
$C_2H_4O_2$	methyl formate	305.14	l	SEL	-970.10	0.86	-388.50	0.86	28.58	0.20	TN	2021RUS
		305.14	g	SEL1	-998.68	0.84	-359.92	0.84			TN	2021RUS
$C_4H_8O_2$	ethyl acetate	350.21	l	SEL	-2237.35	0.46	-479.86	0.46	35.15	0.21	H2O	1991WIB2

		350.21	g	SEL1	-2272.49	0.51	-444.72	0.51			H2O	1991WIB2
$C_4H_6O_2$	vinyl acetate	345.33	l	SEL	-2080.6	2.0	-350.8	2.0	37.15	0.84	H2	1980VIL
		345.33	g	SEL1	-2117.7	2.2	-313.6	2.2			DvH	1980VIL
$C_5H_8O_2$	ethyl acrylate	372.59	l	SEL	-2740.1		-370.6				H2	1980VIL
		372.59	g	SEL1	-2779.3		-331.4				DvH	1980VIL
		372.59	lg	SEL					39.20		v	1975VIL
	methyl methacrylate	369.73	l	SEL	-2728.3	4.0	-382.4	4.0				1980VIL
		369.73	g	SEL1	-2768.3	4.0	-342.3	4.0				1980VIL
Oxacyclohydrocarbons												
C_2H_4O	oxirane	283.59	g	SEL	-1306.00	0.37	-52.60	0.37			TN	2021RUS
		283.59	l	SEL1	-1281.07	0.44	-77.53	0.44	24.93	0.24	TN	2021RUS
C_4H_4O	furan	304.51	l	SEL	-2083.5	0.6	-62.0	0.6	27.60	0.20	C	1952GUT
		304.51	g	SEL1	-2111.1	0.6	-34.4	0.6			DvH	1952GUT
$C_3H_6O_3$	1,3,5-trioxane	335.65	s	SEL	-1515.70	0.30	-522.21	0.30			C	1969MAN
		387.20	l	SEL1	-1526.4	4.8	-511.5	4.8			DfusH	1969MAN
		387.20	g	SEL2	-1572.3	0.5	-465.6	0.5			DsubH	1969MAN
		335.65	s	SEL	-1514.7	0.5	-523.2	0.5	10.73	0.20	f	2019DIK
		387.20	sg	SEL					56.60	0.20	s	1969MAN
$C_4H_8O_2$	1,3-dioxane	378.13	l	SEL	-2339.86	0.99	-377.35	0.99	39.09	0.05	C	1982BYS
		378.13	g	SEL1	-2378.95	0.99	-338.26	0.99			DvH	1982BYS
	1,4-dioxane	374.25	l	SEL	-2362.23	0.99	-354.98	0.99	38.64	0.05	C	1982BYS
		374.25	g	SEL1	-2362.28	0.99	-354.93	0.99			DvH	1982BYS
$C_{10}H_{16}O$	D-camphor	451.8	s	SEL	-5902.0	3.0	-319.4	3.0			C	1977STE
		493.00	g	SEL1	-5953.9	3.1	-267.5	3.1			DsubH	1977STE
		451.8	l	SEL2	-5908.8	3.2	-312.5	3.2			DvH	1977STE
		493.00	lg	SEL					6.82		v	1995CHI
		451.8	sg	SEL					51.88	0.84	s	1977STE
$C_4H_2O_3$	2,5-furandione	325.65	s	SEL	-1389.50	0.67	-470.23	0.67			C	1964WIL
		478.33	g	SEL1	-1458.5	2.1	-401.2	2.1			DvH	1964WIL
		478.33	l	SEL2	-1401.0	2.1	-458.8	2.1			DfusH	1964WIL
		478.33	l	SEL	-1400	10	-459	10	57.5	9.5	v	2019DIK
		325.65	s	SEL	-1389.8	1.1	-470.0	1.1	10.68		f	2019DIK

Aromatic Alcohols												
C_6H_6O	phenol	314.15	s	SEL	-3055.98	0.65	-162.35	0.65	69.01	0.30	TN	2021RUS
		454.91	g	SEL1	-3124.99	0.63	-93.34	0.63			TN	2021RUS
		454.91	l	SEL2	-3071.06	0.70	-147.28	0.70			DfusH	2021RUS
C_7H_8O	3-methylphenol	475.28	l	SEL	-3703.89	0.59	-193.75	0.59	61.71	1.05	C	1960AND
		475.28	g	SEL1	-3765.6	1.2	-132.0	1.2			DvH	1960AND
		285.37	s	SEL2	-3693.18	0.78	-204.46	0.78			DfusH	1960AND
		285.37	sl	SEL					10.71		f	1996DOM
	benzyl alcohol	478.50	l	SEL	-3736.9	1.3	-160.7	1.3			C	1954PAR
		478.50	g	SEL1	-3801.7	1.4	-95.9	1.4			DvH	1954PAR
		478.50	lg	SEL					64.80	0.60	v	1999VER
Oxa-Aromatics												
C_7H_6O	benzaldehyde	451.15	l	SEL	-3525.01	1.10	-86.80	1.10	49.73	0.40	TN	2021RUS
		451.15	g	SEL1	-3574.74	0.91	-37.07	0.91			TN	2021RUS
$C_7H_6O_2$	benzoic acid	395.50	s	SEL	-3227.01	0.18	-384.80	0.17			TN	2021RUS
		523.53	g	SEL1	-3317.62	0.21	-294.19	0.20	90.61	0.50	TN	2021RUS
		523.53	l	SEL2	-3238.72	0.21	-373.09	0.20			DvH	2021RUS
		523.53	lg	SEL					78.90		v	1995CHI
		395.50	sg	SEL					89.30	0.50	s	1990SIL

Table 4-4(5). Nitrogen-Substituted Hydrocarbons

Formula	Compound	T_{trs} [K]	Ph	SEL	$\Delta_c H$	*u*	$\Delta_f H$	*u*	$\Delta_{trs} H$	*u*	M	R	Ref
					kJ mol^{-1}								
Hydrogen Cyanide													
CHN	hydrogen cyanide	298.79	l	SEL	-639.08	0.30	102.69	0.30			DvH		2021RUS
		298.79	g	SEL1	-665.669	0.092	129.280	0.089			TN		2021RUS
		298.79	g	SEL	-665.4	2.7	129.0	2.7	26.59	0.29	v		2019DIK
Alkylamines													
CH_5N	methylamine	266.84	g	SEL	-1086.81	0.24	-21.23	0.24			TN		2021RUS
		266.84	l	SEL1	-1062.79	0.45	-45.25	0.45	24.02	0.30	TN		2021RUS
C_2H_7N	ethylamine	289.79	g	SEL	-1737.31	0.54	-50.03	0.54			TN		2021RUS
		289.79	l	SEL1	-1713.25	0.55	-74.09	0.55	24.06		TN		2021RUS
C_3H_9N	1-propylamine	320.38	l	SEL	-2365.13	0.41	-101.52	0.41	31.42	0.15	TN		2021RUS
		320.38	g	SEL1	-2396.55	0.42	-70.10	0.42			TN		2021RUS
	isopropylamine	304.92	l	SEL	-2354.37	0.52	-112.28	0.52	28.71	0.20	TN		2021RUS
		304.92	g	SEL1	-2383.08	0.53	-83.57	0.53			TN		2021RUS
$C_4H_{11}N$	n-butylamine	350.12	l	SEL	-3018.46	1.13	-127.48	1.13	32.64	1.26	C		1959EVA
		350.12	g	SEL1	-3054.17	1.13	-91.77	1.13			DvH		1959EVA
		350.12	lg	SEL					35.71	0.06	v		1969WAD
C_2H_7N	dimethylamine	280.02	g	SEL	-1769.79	0.42	-17.55	0.42			TN		2021RUS
		280.02	l	SEL1	-1743.91	0.37	-43.43	0.37	25.88	0.20	TN		2021RUS
C_3H_9N	methylethylamine	305.60	l	SEL	-2391.4	2.3	-75.2	2.3			TN		2021RUS
		305.60	g	SEL1	-2420.7	1.1	-45.9	1.1			TN		2021RUS
	trimethylamine	276.00	g	SEL	-2439.91	0.76	-26.74	0.76			TN		2021RUS
		276.00	l	SEL1	-2417.80	0.87	-48.85	0.87	22.11	0.10	TN		2021RUS
$C_6H_{15}N$	triethylamine	361.93	l	SEL	-4377.09	0.54	-127.46	0.55			C		1966LEB
		361.93	g	SEL1	-4412.49	0.59	-92.06	0.58			DvH		1966LEB
		361.93	lg	SEL					35.40	0.20	v		2009MOK
$C_6H_{13}N$	cyclohexylamine	406.98	l	SEL	-4071.3	1.3	-147.4	1.3			C		1979STE
		406.98	g	SEL1	-4113.8	1.3	-104.9	1.3			DvH		1979STE
		406.98	lg	SEL					42.80	0.10	v		1975BER

Alkanenitriles												
C_2H_3N	ethanenitrile	355.05	l	SEL	-1256.29	0.22	40.60	0.22	33.45	0.21	TN	2021RUS
		355.05	g	SEL1	-1289.74	0.25	74.05	0.25			TN	2021RUS
C_3H_5N	propanenitrile	370.73	l	SEL	-1910.62	0.54	15.63	0.55	35.98		C	1971HAL
		370.73	g	SEL1	-1946.60	0.62	51.61	0.62			C	1971HAL
C_4H_7N	butanenitrile	390.77	l	SEL	-2568.68	0.92	-5.61	0.92	36.99		C	1959EVA
		390.77	g	SEL1	-2605.67	0.92	31.37	0.95			DvH	1959EVA
C_3H_3N	propenenitrile	351.13	l	SEL	-1756.40	0.42	147.23	0.42	32.64		C	1971HAL
		351.13	g	SEL1	-1789.04	0.72	179.87	0.72			DvH	1971HAL
Azahydrocarbons												
C_2N_2	cyanogen	252.00	g	SEL	-1097.07	0.41	310.12	0.41			TN	2021RUS
		252.00	l	SEL1	-1076.13	0.42	289.18	0.42	20.94		TN	2021RUS
$C_2H_8N_2$	1,1-dimethylhydrazine	335.57	l	SEL	-1978.7	3.6	48.4	3.6			C	1960DON
		335.57	g	SEL1	-2013.7	3.6	83.4	3.6			DvH	1960DON
		335.57	l	SEL					35.00	0.17	v	1952AST
$C_3H_6N_6$	1,3,5-triazine-2,4,6-triamine	618	s	SEL	-1972.0	3.0	-65.9	3.0			C	1973SEL
C_6H_7N	aniline	457.30	l	SEL	-3393.06	0.84	31.81	0.84	55.77		C	1962HAT
		457.30	g	SEL1	-3448.27	0.88	87.03	0.88			DvH	1962HAT
$C_8H_{11}N$	*N*,*N*-dimethylaniline	466.47	l	SEL	-4767.8	3.2	47.9	3.2	52.83	0.03	C	1982FUR
		466.47	g	SEL1	-4820.6	3.2	100.8	3.2			DvH	1982FUR
		275.65	s	SEL2	-4756.2	3.2	36.4	3.2			DfusH	1982FUR
		275.65	sl	SEL					11.56		f	1972AHN
$C_6H_{15}NO_3$	triethanolamine	623.15	l	SEL	-3840.6	1.5	-664.0	1.5	105.9	2.2	C	1982MIN
		623.15	g	SEL1	-3946.3	2.7	-558.3	2.7			DvH	1982MIN
Nitroalkanes and Nitrites												
CH_3NO_3	methyl nitrate	338.00	g	SEL	-700.0	1.3	-122.2	1.3			E	1959RAY
CN_4O_8	tetranitromethane	397.95	l	SEL	-431.8	1.7	38.3	1.7	43.93	0.42	C	1975LEB
		397.95	g	SEL1	-475.7	1.7	82.2	1.7			DvH	1975LEB
		287.05	s	SEL2	-395.4	4.3	1.9	4.3			DfusH	1975LEB
		287.05	sl	SEL					36.4	4.0	f(est)	2021CHE
CH_3NO_2	nitromethane	374.34	l	SEL	-709.25	0.43	-112.97	0.43	38.26	0.10	TN	2021RUS
		374.34	g	SEL1	-747.51	0.46	-74.71	0.46			TN	2021RUS

$C_9H_6N_2O_2$	2,4-diisocyanatotoluene	524.83	l	SEL	-4235.0		-163.7		49.5		C	1962STR
		524.83	g	SEL1	-4284.5		-114.2				DvH	1962STR
		293.65	s	SEL2	-4168.0		-230.8				est	1985CHR
		524.83	lg	SEL					49.5	5.2	v	2019DIK
$C_6H_5NO_2$	nitrobenzene	483.81	l	SEL	-3082.0	1.4	6.6	1.4	55.00	0.05	TN	2021RUS
		483.81	g	SEL1	-3137.0	1.4	61.6	1.4			TN	2021RUS
$C_7H_5N_3O_6$	trinitrotoluene	355.10	s	SEL	-3406.0	3.0	-62.9	3.0			C	1976ROU
		621.00	g	SEL1	-3519.2	3.4	50.3	3.4			DsubH	1976ROU
		621.00	l	SEL2	-3493.0	3.6	24.1	3.6			DvH	1976ROU
		621.00	lg	SEL					87.00	1.90	v	1978CUN
		355.10	sg	SEL					113.20	1.50	s	1979KUD

Table 4-4(6). Sulfur-Substituted Hydrocarbons

Formula	Compound	T_{trs} [K]	Ph	SEL	$\Delta_c H$	u	$\Delta_f H$ kJ mol^{-1}	u	$\Delta_{trs} H$	u	M	R	Ref
Akanethiols													
CH_4S	methanethiol	279.05	g	SEL	-1544.57	0.51	-22.55	0.51			DvH		1961GOO
		279.05	l	SEL1	-1520.8	0.5	-46.35	0.5	23.81	0.08	R	a	1961GOO
C_2H_6S	ethanethiol	308.19	l	SEL	-2173.17	0.42	-73.68	0.42			C	a	1957MCC
		308.19	g	SEL1	-2200.3	0.43	-46.1	0.43			DvH		1957MCC
Sulfides													
CS_2	carbon disulfide	318.35	l	SEL	-1687.2	0.5	89.71				C	a	1961GOO
		318.35	g	SEL1	-1714.5	0.5	117.1				DvH		1961GOO
C_2H_6S	dimethyl sulfide	310.42	l	SEL	-2181.45	0.33	-64.96				C	a	1957MCC
		310.42	g	SEL1	-2208.8	0.59	-37.57	0.59			DvH		1957MCC
C_2H_6OS	dimethyl sulfoxide	463.86	l	SEL	-2037.30	1.25	-203.40		52.90	0.83	C	g	1994MAS
		463.86	g	SEL1	-2095.9	1.5	-150.5	1.5			DvH		1994MAS

Table 4-4(7). Halogenated Hydrocarbons

Formula	Compound	T_{trs} [K]	Ph	SEL	$\Delta_c H$	*u*	$\Delta_f H$ kJ mol^{-1}	*u*	$\Delta_{trs} H$	*u*	M	R	Ref
Fluoroalkanes													
CH_3F	fluoromethane	194.65	g	SEL	-764.86	0.28	-235.49	0.23			TN	k	2021RUS
		194.65	l	SEL1	-756.33	1.15	-244.02	1.14			DvH		2021RUS
		194.65	lg	SEL					8.53	1.12	v		2019DIK
CH_2F_2	difluoromethane	221.50	g	SEL	-584.82	0.40	-450.76	0.33			TN	k	2021RUS
		221.50	l	SEL1	-566.84	0.43	-468.74	0.36	17.98	0.20	TN		2021RUS
CHF_3	trifluoromethane	188.75	g	SEL	-374.80		-696.00	0.41			TN	k	2021RUS
		188.75	l	SEL1	-366.34		-704.46	0.43	8.46	0.30	TN		2021RUS
CF_4	tetrafluoromethane	145.56	g	SEL	-172.55		-933.47	0.25			TN	k	2021RUS
		145.56	l	SEL1	-160.74		-945.28	0.56			DvH		2021RUS
		145.56	lg	SEL					11.81		v		1969SMI
C_2H_5F	fluoroethane	236.05	g	SEL	-1407.52	0.40	-272.13	0.36			TN		2021RUS
		236.05	l	SEL1	-1391.21	0.47	-288.45	0.44			DvH		2021RUS
		236.05	lg	SEL					16.32	0.25	v		2019DIK
$C_2H_4F_2$	1,1-difluoroethane	249.13	g	SEL	-1212.14	0.60	-502.74	0.55			DvH		2021RUS
		249.13	l	SEL1	-1193.66	0.88	-521.22	0.84			TN		2021RUS
	1,2-difluoroethane	293.00	g	SEL	-1267.04	0.84	-447.84	0.81			TN		2021RUS
		293.00	l	SEL1	-1245.91	0.98	-468.97	0.95	21.13	0.50	DvH		2021RUS
		293.00	lg	SEL					21.13	0.50	v		2022BUR1
$C_2H_3F_3$	1,1,1-trifluoroethane	225.91	g	SEL	-1008.3	1.7	-748.5	1.7			C		1965KOL
		225.91	l	SEL1u	-988.2	2.0	-761.9	1.9			DvH		1965KOL
		225.91	lg	SEL					13.43	0.97	v		2019DIK
	1,1,2-trifluoroethane	276.81	g	SEL	-1059	10	-691	10			H2		1965KOL
		276.81	l	SEL1	-1035	10	-715	10			DvH		1965KOL
		276.81	lg	SEL					24.28	0.45	v		2019DIK
$C_2H_2F_4$	1,1,1,2-tetrafluoroethane	247.08	g	SEL	-883.7	2.0	-901.6	2.0			CBS		1988BER
		247.08	l	SEL1	-865.6	2.0	-919.7	2.0	18.10	0.16	DvH		1988BER
		247.08	lg	SEL					18.10	0.16	v		2019DIK
	1,1,2,2-tetrafluoroethane	253.23	g	SEL	-910.1	2.0	-875.2	2.0			CBS		1988BER
		253.23	l	SEL1	-890.3	2.3	-895.0	2.3			G3B3		2016GOO
		253.23	lg	SEL					19.79	1.13	v		2019DIK
C_2HF_5	pentafluoroethane	225.06	g	SEL	-701	8	-1120	8			G3B3		2016GOO
		225.06	l	SEL1	-687	8	-1133	8			DvH		2016GOO

		225.06	lg	SEL					13.44	0.16	v	2019DIK
C_2F_6	hexafluoroethane	194.87	g	SEL	-513.33		-1342.44	0.97			TN	2021RUS
		194.87	l	SEL1	-506.33		-1349.44	1.09	7.00	0.50	DvH	2021RUS
		194.87	lg	SEL					7.00	0.50	v	2022BUR1
Fluoroalkenes												
$C_2H_3F_3$	fluoroethene	201.65	g	SEL	-1251.41	0.48	-142.42	0.45			TN	2021RUS
		201.65	l	SEL1	-1240.61	0.90	-153.22	0.88			DvH	2021RUS
$C_2H_3F_3$		201.65	l	SEL	-1244.0	3.3	-149.8	3.3	10.80	0.76	v	2019DIK
$C_2H_2F_2$	1,1-difluoroethene	190.15	g	SEL	-1078.41	0.80	-350.64	0.77			TN	2021RUS
		190.15	l	SEL1	-1074.0	2.7	-355.1	2.7			DvH	2021RUS
		190.15	lg	SEL	-1090.5	4.3	-338.6	4.3	4.4	2.6	v	2019DIK
	1,2-difluoroethene, (E)-	231.15	g	SEL	-1123.0	0.9	-306.1	0.9			TN	2021RUS
		231.15	l	SEL1	-1108.05	1.39	-321.00	1.38			DvH	2021RUS
		231.15	lg	SEL					14.90	1.04	v	2019DIK
	1,2-difluoroethene, (Z)-		g	SEL	-1119.4	0.9	-309.7	0.9			TN	2021RUS
		253.15	l	SEL1	-1105.6	1.3	-323.4	1.3			DvH	2021RUS
		253.15	lg	SEL					13.79	0.94	v	2019DIK
C_2HF_3	trifluoroethene	211.70	g	SEL	-966.2	1.6	-498.1	1.6			TN	2021RUS
		211.70	l	SEL1	-954.8	1.9	-509.5	1.8			DvH	2021RUS
		211.70	lg	SEL					11.37	0.92	v	2019DIK
C_2F_4	tetrafluoroethene	197.51	g	SEL	-825.10	0.61	-674.40	0.52			TN	2021RUS
		197.51	l	SEL1	-819.00	1.44	-680.50	1.40			DvH	2021RUS
		197.51	lg	SEL	-844	23	-656	23	6.10	1.30	v	2019DIK
Chlorolakenes												
CH_3Cl	chloromethane	249.00	g	SEL	-763.51	0.39	-82.24	0.39			TN	2021RUS
		249.00	l	SEL1	-743.61	0.25	-102.14	0.25	19.90	0.30	TN	2021RUS
CH_2Cl_2	dichloromethane	312.92	g	SEL	-633.00	0.52	-93.38	0.52			TN	2021RUS
		312.92	l	SEL1	-603.99	0.54	-122.39	0.54	29.01	0.10	TN	2021RUS
$CHCl_3$	trichloromethane	334.42	g	SEL	-504.94	0.50	-102.07	0.50			TN	2021RUS
		334.42	l	SEL1	-473.54	0.51	-133.47	0.51	31.40	0.10	TN	2021RUS
CCl_4	tetrachloromethane	349.65	g	SEL	-392.02	0.43	-95.61	0.43			TN	2021RUS
		349.65	l	SEL1	-359.52	0.43	-128.11	0.43	32.5		TN	2021RUS
C_2H_5Cl	chloroethane	285.40	g	SEL	-1413.57	0.26	-111.49	0.26			TN	2021RUS
		285.40	l	SEL1	-1389.14	0.40	-135.92	0.40	24.43	0.30	TN	2021RUS
$C_2H_4Cl_2$	1,1-dichloroethane	330.42	g	SEL	-1272.61	0.44	-133.07	0.44			TN	2021RUS
		330.42	l	SEL1	-1241.81	0.48	-163.87	0.48	30.8		TN	2021RUS
	1,2-dichloroethane	356.70	l	SEL	-1238.5	3.5	-167.2	3.5	35.21	0.05	R	2002MAN

		356.70	g	SEL1	-1273.7	3.5	-132.0	3.5			R	2002MAN
$C_2H_3Cl_3$	1,1,1-trichloroethane	347.22	l	SEL	-1109.1	2.0	-177.2	2.0	32.59	0.07	R	2002MAN
		347.22	g	SEL1	-1141.7	2.0	-144.6	2.0			R	2002MAN
	1,1,2-trichloroethane	386.78	l	SEL	-1098.0	4.0	-188.3	4.0	40.30	0.07	R	2002MAN
		386.78	g	SEL1	-1138.3	4.0	-148.0	4.0			R	2002MAN
$C_2H_2Cl_4$	1,1,1,2-tetrachloroethane	403.33	l	SEL	-973.5	2.3	-193.4	2.3	41.10	0.50	R	2002MAN
		403.33	g	SEL1	-1014.6	2.4	-152.3	2.4			R	2002MAN
	1,1,2,2-tetrachloroethane	419.25	l	SEL	-964.5	3.5	-202.4	3.5	45.73	0.09	R	2002MAN
		419.25	g	SEL1	-1010.2	3.5	-156.7	3.5			R	2002MAN
C_2HCl_5	pentachloroethane	433.45	l	SEL	-844.3	4.0	-203.3	4.0	47.40	1.50	R	2002MAN
		433.45	g	SEL1	-891.7	4.3	-155.9	4.3			R	2002MAN
C_2Cl_6	hexachloroethane	462.96	l	SEL	-711.7	2.8	-216.5	2.8	67.1		TN	2021RUS
		462.96	g	SEL1	-778.8	1.3	-149.4	1.3			TN	2021RUS
Chloroalkenes												
C_2H_3Cl	chloroethene	259.35	l	SEL	-1241.13	0.36	1.90	0.36	19.80	0.20	TN	2021RUS
		259.35	g	SEL1	-1260.93	0.30	21.70	0.30			TN	2021RUS
$C_2H_2Cl_2$	1,1-dichloroethene	304.71	l	SEL	-1122.81	0.49	2.95	0.49	26.75	0.15	TN	2021RUS
		304.71	g	SEL1	-1096.06	0.50	-23.80	0.50			TN	2021RUS
	1,2-dichloroethene, (E)-	320.73	l	SEL	-1119.74	0.54	-0.12	0.54			DvH	2021RUS
		320.73	g	SEL1	-1149.24	1.14	29.38	1.14			TN	2021RUS
		320.73	lg	SEL					29.50	1.00	v	2002MAN
	1,2-dichloroethene, (Z)-	333.58	l	SEL	-1086.23	1.14	-33.63	1.14			TN	2021RUS
		333.58	g	SEL1	-1117.33	0.54	-2.53	0.54			TN	2021RUS
C_2HCl_3	trichloroethene	360.50	l	SEL	-985.9	1.5	-14.6	1.5	34.60	0.15	TN	2021RUS
		360.50	g	SEL1	-951.3	1.5	-49.2	1.5			TN	2021RUS
C_2Cl_4	tetrachloroethene	394.29	l	SEL	-818.2	1.1	-62.9	1.1	39.70	0.10	TN	2021RUS
		394.29	g	SEL1	-857.9	1.1	-23.2	1.1			TN	2021RUS
Chloroalkynes												
C_2HCl	chloroethyne	243.6	g	SEL	-1182.39	0.70	228.99	0.70			TN	2021RUS
		243.6	l	SEL1	-1162.4	1.2	209.0	1.2			DvH	2021RUS
		243.6	lg	SEL					20.0	1.0	v	2002MAN
		306.00	lg	SEL					27.4	1.2	v	2002MAN
Bromoalkanes												
CH_3Br	bromomethane	276.70	g	SEL	-763.80	0.26	-35.61	0.26			TN	2021RUS
		276.70	l	SEL1	-740.47	0.27	-58.94	0.27			TN	2021RUS
CH_2Br_2	dibromomethane	370.10	l	SEL	-601.3	1.1	-32.4	1.1			TN	2021RUS
		370.10	g	SEL1	-638.3	1.1	4.6	1.1			TN	2021RUS

$CHBr_3$	tribromomethane	422.36	l	SEL	-471.5	1.3	3.5	1.3	46.10	0.10	TN	2021RUS
		422.36	g	SEL1	-517.6	1.3	49.6	1.3			TN	2021RUS
CBr_4	tetrabromomethane	462.55	l	SEL	-351.6	1.4	49.3	1.4			TN	2021RUS
		462.55	g	SEL1	-406.1	1.3	103.8	1.3			TN	2021RUS
		462.55	sg	SEL					54.50	0.70	s	1984BIC
C_2H_5Br	bromoethane	311.54	l	SEL	-1387.66	0.26	-91.05	0.26			TN	2021RUS
		311.54	g	SEL1	-1415.65	0.25	-63.06	0.25			TN	2021RUS
Bromoethenes												
C_2H_3Br	bromoethene	288.60	g	SEL	-1266.79	0.57	73.90	0.57			TN	2021RUS
		288.60	l	SEL1	-1233.0	1.8	40.1	1.8			DvH	2021RUS
		288.60	lg	SEL					33.76	1.74	v	2019DIK
Chlorofluoroalkanes												
CH_2ClF	chlorofluoromethane	264.00	g	SEL	-617.7	1.1	-263.3	1.1			TN	2021RUS
		264.00	l	SEL1	-599.1	1.5	-281.9	1.5			DvH	2021RUS
		264.00	lg	SEL					18.62	0.96	v	2019DIK
$CHClF_2$	chlorodifluoromethane	232.35	g	SEL	-433.99	1.01	-482.21	0.98			TN	2021RUS
		232.35	l	SEL1	-418.29	1.05	-497.91	1.03			DvH	2021RUS
		232.35	lg	SEL					15.70	0.24	v	2019DIK
$CHCl_2F$	dichlorofluoromethane	282.05	g	SEL	-478.01	0.92	-283.59	0.91			TN	2021RUS
		282.05	l	SEL1	-454.4	1.5	-307.2	1.5			DvH	2021RUS
		282.05	lg	SEL					23.64	1.18	v	2019DIK
$CClF_3$	chlorotrifluoromethane	191.75	g	SEL	-241.78	0.63	-709.65	0.57			TN	2021RUS
		191.75	l	SEL1	-225.28	0.70	-726.15	0.64			TN	2021RUS
CCl_2F_2	dichlorodifluoromethane	243.35	g	SEL	-303.18	0.71	-493.65	0.67			TN	2021RUS
		243.35	l	SEL1	-286.38	0.73	-510.45	0.70			DvH	2021RUS
		243.35	lg	SEL					16.80	0.23	v	2019DIK
CCl_3F	trichlorofluoromethane	296.95	g	SEL	-353.80	0.80	-288.43	0.78			TN	2021RUS
		296.95	l	SEL1	-329.01	0.81	-313.22	0.80			TN	2021RUS
C_2ClF_3	chlorotrifluoroethene	244.80	g	SEL	-833.2	2.8	-511.7	4.7			DvH	1982ERA
		244.80	l	SEL1	-816.0	2.8	-528.9	2.8	17.2	3.8	C	1982ERA
Bromofluoroalkanes												
CH_2BrF	bromofluoromethane	310.00	l	SEL	-591.3	5.2	-243.4	5.2			DvH	2021RUS
		310.00	g	SEL1	-622.7	4.9	-211.9	4.9			TN	2021RUS
		310.00	lg	SEL					31.47	1.72	v	2019DIK
$CHBrF_2$	bromodifluoromethane	258.65	g	SEL	-445.5	1.2	-424.3	1.2			TN	2021RUS
		258.65	l	SEL1	-425.5	1.6	-444.4	1.5			DvH	2021RUS
		258.65	lg	SEL					20.02	0.96	v	2019DIK

$CHBr_2F$	dibromofluoromethane	338.05	l	SEL	-456.9	5.2	-212.0	5.2			DvH	2021RUS
		338.05	g	SEL1	-489.6	4.9	-179.3	4.9			TN	2021RUS
		338.05	lg	SEL					32.73	1.81	v	2019DIK
$CBrF_3$	bromotrifluoromethane	215.35	g	SEL	-254.08	0.52	-651.00	0.44			TN	2021RUS
		215.35	l	SEL1	-242.31	0.53	-662.78	0.46			TN	2021RUS
CBr_2F_2	dibromodifluoromethane	297.65	g	SEL	-322.1	1.3	-382.0	1.3			TN	2021RUS
		297.65	l	SEL1	-297.7	1.3	-406.4	1.3			DvH	2021RUS
		297.65	lg	SEL					24.42	0.19	v	2019DIK
CBr_3F	tribromofluoromethane	379.65	l	SEL	-324.4	3.0	-178.9	3.0			DvH	2021RUS
		379.65	g	SEL1	-373.7	1.5	-129.5	1.5			TN	2021RUS
		379.65	lg	SEL					49.4	2.6	v	2019DIK
Bromochloroalkanes												
CH_2BrCl	bromochloromethane	341.21	l	SEL	-605.1	1.3	-74.9	1.3			DvH	2021RUS
		341.21	g	SEL1	-637.8	1.3	-42.2	1.3			TN	2021RUS
		341.21	lg	SEL					32.75	0.18	v	2019DIK
$CHBrCl_2$	bromodichloromethane	362.65	l	SEL	-476.6	2.2	-84.1	2.2			DvH	2021RUS
		362.65	g	SEL1	-511.6	1.2	-49.1	1.2			TN	2021RUS
		362.65	lg	SEL					35.01	1.84	v	2019DIK
$CHBr_2Cl$	dibromochloromethane	393.00	l	SEL	-470.4	4.1	-44.0	4.1			DvH	2021RUS
		393.00	g	SEL1	-514.3	3.4	0.0	3.4			TN	2021RUS
		393.00	lg	SEL					44.0	2.3	v	2019DIK
$CBrCl_3$	bromotrichloromethane	376.65	l	SEL	-363.8	1.6	-77.5	1.6			DvH	2021RUS
		376.65	g	SEL1	-399.40	0.59	-41.89	0.59			TN	2021RUS
		376.65	lg	SEL					35.64	1.49	v	2019DIK
CBr_2Cl_2	dibromodichloromethane	423.35	l	SEL	-360.5	4.2	-34.4	4.2	-39.5		DvH	2021RUS
		423.35	g	SEL1	-400.0	1.3	5.1	1.3			TN	2021RUS
		423.35	lg	SEL					39.5	4.0	v	2019DIK
CBr_3Cl	tribromochloromethane	433.00	l	SEL	-355.0	2.9	6.4	2.9			DvH	2021RUS
		433.00	g	SEL1	-403.0	1.5	54.4	1.5			TN	2021RUS
		433.00	lg	SEL					48.1	2.5	v	2019DIK
Bromochlorofluoroalkanes												
CHBrClF	bromochlorofluoromethane	312.60	l	SEL	-456.7	5.1	-258.5	5.1	27.6		DvH	2021RUS
		312.60	g	SEL1	-484.4	4.9	-230.9	4.9			TN	2021RUS
		312.60	lg	SEL					27.62	1.52	v	2019DIK
$CBrClF_2$	bromochlorodifluoromethane	270.65	g	SEL	-310.6	4.9	-439.9	4.9			TN	2021RUS
		270.65	l	SEL1	-289.9	4.9	-460.6	4.9			DvH	2021RUS
		270.65	lg	SEL					20.72	0.12	v	2019DIK

$CBrCl_2F$	bromodichlorofluoromethane	325.15	l	SEL	-326.8	5.2	-269.1	5.2			DvH	2021RUS
		325.15	g	SEL1	-357.6	4.9	-238.3	4.9			TN	2021RUS
		325.15	lg	SEL					30.78	1.70	v	2019DIK
CBr_2ClF	dibromochlorofluoromethane	352.65	l	SEL	-327.2	5.2	-222.3	5.2			DvH	2021RUS
		352.65	g	SEL1	-362.7	4.9	-186.8	4.9			TN	2021RUS
		352.65	l	SEL					35.51	1.93	v	2019DIK
Carbonyl Halides												
CCl_2O	phosgene	280.71	g	SEL	-221.41	0.27	-219.14	0.27			TN	2021RUS
		280.71	l	SEL1	-198.58	0.47	-241.98	0.47			DvH	2021RUS
		280.71	l	SEL	-197.60	0.39	-242.96	0.39	22.84	0.39	v	2019DIK
Pentachlorophenol												
C_6HCl_5O	pentachlorophenol	463.84	s	SEL	-2329.0	2.9	-292.5	3.0			C	1958SIN
		582.50	l	SEL1	-2346.1	3.0	-275.4	3.0			DsubH	1958SIN
		582.50	g	SEL2	-2420.6	3.0	-200.9	3.0			DvH	1958SIN
		582.50	sg	SEL					91.60	0.50	s	2007VER
		463.84	sl	SEL					17.15	0.50	v	1991ACR

Table 4-4(8). Recommended Gross and Net Heats of Combustion

This table contains both recommended gross $\Delta_c H$ and net $\Delta_c H$(net) heats of combustion. Gross heats of combustion are where the products are at standard state (298.15 K and 1 bar) where water is in the liquid phase, while net heats of combustion are where the products are all gaseous. The recommended gross heats of combustion are the same as those provided in the previous Tables 4-4(1-7). The compounds in this table are organized by primary and secondary compound class and then by molecular formula.

Formula	Compound	T_{trs} [K]	Ph	SEL	$\Delta_c H$	$\Delta_c H$(net) kJ mol^{-1}	*u*	M	R	Ref
SMALL MOLECULES										
Hydrogen/Oxygen										
H_2	Hydrogen	20.37	g	SEL	-285.826	-241.832	0.000	def		def
O_2	Oxygen	90.19	g	SEL	0.000	0.000	0.000	def		def
H_2O_2	hydrogen peroxide	426.40	l	SEL	-98.48	-54.49	0.79	TN		2021RUS
		426.40	g	SEL1	-150.368	-106.374	0.068	TN		2021RUS
		272.74	s	SEL2	-86.26	-42.27	0.79	DfusH		1955GIG
H_2O	Water	373.12	l	SEL	0.000	43.994	0.037	TN		2021RUS
		373.12	g	SEL1	-43.994	0.000	0.037	TN		2021RUS
		273.153	s	SEL2	6.913	50.907	0.037	TN		2021RUS
Nitrogen/Hydrogen										
N_2	nitrogen	77.36	g	SEL	0.000	0.000	0.000	def		
H_3N	ammonia	239.82	g	SEL	-383.181	-317.190	0.029	TN		2021RUS
		239.82	l	SEL1	-363.32	-297.33	0.11	DvH		2021RUS
ClH_4NO_4	ammonium perchlorate	403.15	s(d)	SEL	-442.33	-280.07	0.17			1998CHA
H_4N_2	hydrazine	386.65	l	SEL	-622.34	-534.35				2021RUS
		386.65	g	SEL1	-669.22	-581.23				2021RUS
Hydrogen Halides										
FH	hydrogen fluoride	292.7	g	SEL	na	na		TN		2021RUS
		292.7	l	SEL1	na	na		TN		2021RUS
	hydrogen fluoride (aq, 20 H_2O)	292.7	aq	SEL	na	na		TN		2021RUS
ClH	hydrogen chloride	188.1	g	SEL	na	na		TN		2021RUS
	hydrogen chloride (aq, 600 H_2O)	188.1	aq	SEL	na	na		TN		2021RUS
BrH	hydrogen bromide	206.77	g	SEL	na	na		R		1984COX
	hydrogen bromide (aq, 600 H_2O)	206.77	aq	SEL	na	na		TN		2021RUS
Sulfur/Hydrogen/Oxygen										
H_2S	hydrogen sulfide	212.85	g	SEL	-867.21	-759.87	0.5	R		1984COX
		212.85	l	SEL1	-853.55	-504.38	0.64	DvH		1984COX

O_2S	sulfur dioxide	263.14	l	SEL	na	na		R	1982WAG
		263.14	g	SEL1	na	na		R	1982WAG
H_2O_4S	sulfuric acid	283.46	l	SEL1	na	na		R	1982WAG
		283.46	g	SEL2	na	na		R	1998CHA
	sulfuric acid (aq, 115 H_2O)	283.46	aq	SEL	na	na		R	1982WAG
Boron Compounds									
BH_3O_3	boric acid	444.05	s	SEL	na	na		D	1950SMI
	boric acid (aq, 500 H_2O)	444.05	aq	SEL	na	na		H2O	1950SMI
B_2H_6	diborane	180.59	g	SEL	-2175.76	-2043.79	1.17	D	1965GUN
		180.59	l	SEL1	-2174.75	-2042.78	1.17	DvH	1965GUN
B_2O_3	diboron trioxide	723.15	s	SEL	na	na			1959JOH
		2130	g	SEL1	na	na			1963HIL
		2130	l	SEL2	na	na			1961NBS

HYDROCARBONS									
Carbon									
C	diamond	4300	s	SEL1	-395.347	-395.347	0.070	C	1966HAW
	graphite	4800	s	SEL	-393.476	-393.476	0.025	def	1966HAW
		5000	g	SEL1	-1110.359	-1110.359	0.047	TN	2021RUS
Alkanes									
CH_4	methane	111.67	g	SEL	-890.602	-802.614	0.050	TN	2021RUS
C_2H_6	ethane	184.57	g	SEL	-1560.39	-1428.41	0.13	TN	2021RUS
		184.57	l	SEL1	-1555.58	-1423.60	1.03	DvH	2021RUS
C_3H_8	propane	231.04	g	SEL	-2218.66	-2042.69	0.16	TN	2021RUS
		231.04	l	SEL1	-2203.31	-2027.34	0.26	DvH	2021RUS
C_4H_{10}	isobutane	261.40	g	SEL	-2868.41	-2648.44	0.30	TN	2021RUS
		261.40	l	SEL1	-2848.95	-2628.98	0.37	DvH	2021RUS
	n-butane	272.66	g	SEL	-2877.28	-2657.31	0.24	TN	2021RUS
		272.66	l	SEL1	-2854.88	-2634.91	0.69	DvH	2021RUS
C_5H_{12}	isopentane	300.98	l	SEL	-3503.95	-3239.98	0.43	TN	2021RUS
		300.98	g	SEL1	-3529.17	-3265.20	0.43	TN	2021RUS
	neopentane	282.65	l	SEL	-3492.56	-3228.59	0.39	TN	2021RUS
		282.65	g	SEL1	-3514.95	-3250.98	0.39	TN	2021RUS
	n-pentane	309.21	l	SEL	-3509.35	-3245.38	0.43	TN	2021RUS
		309.21	g	SEL1	-3536.09	-3272.12	0.31	TN	2021RUS
C_6H_{14}	3-methylpentane	336.43	l	SEL	-4159.90	-3851.94	0.88	C	1945PRO
		336.43	g	SEL1	-4190.2	-3882.2	1.0	DvH	1945PRO
	isohexane	333.42	l	SEL	-4157.65	-3849.69	0.83	TN	2021RUS
		333.42	g	SEL1	-4187.76	-3879.80	0.84	TN	2021RUS
	neohexane	322.89	l	SEL	-4148.50	-3840.54	0.88	C	1945PRO
		322.89	g	SEL1	-4176.18	-3868.22	0.96	DvH	1945PRO
	n-hexane	341.87	l	SEL	-4163.04	-3855.08	0.34	TN	2021RUS
		341.87	g	SEL1	-4194.75	-3886.79	0.39	TN	2021RUS
C_7H_{16}	n-heptane	371.55	l	SEL	-4816.83	-4464.88	0.46	TN	2021RUS
		371.55	g	SEL1	-4853.48	-4501.53	0.46	TN	2021RUS
C_8H_{18}	n-octane	398.79	l	SEL	-5470.63	-5074.69	0.55	TN	2021RUS
		398.79	g	SEL1	-5512.16	-5116.22	0.54	TN	2021RUS
C_9H_{20}	n-nonane	423.91	l	SEL	-6124.85	-5684.91	0.50	TN	2021RUS
		423.91	g	SEL1	-6171.29	-5731.35	0.51	TN	2021RUS
$C_{10}H_{22}$	n-decane	447.27	l	SEL	-6778.29	-6294.35	0.80	TN	2021RUS
		447.27	g	SEL1	-6829.68	-6345.74	0.91	TN	2021RUS

$C_{16}H_{34}$	n-hexadecane	559.94	l	SEL	-10699.1	-9951.2	1.8	C	1955FRA
		559.94	g	SEL1	-10780.5	-10032.6	1.8	DvH	1955FRA
Alkenes									
C_2H_4	ethene	169.38	g	SEL	-1410.92	-1322.94	0.12	TN	2021RUS
		169.38	l	SEL1	-1402.48	-1314.50	0.17	DvH	2021RUS
C_3H_6	propene	225.53	g	SEL	-2057.79	-1925.80	0.20	TN	2021RUS
		225.53	l	SEL1	-2043.57	-1911.58	0.33	DvH	2021RUS
C_4H_8	1-butene	266.83	g	SEL	-2717.30	-2541.32	0.36	TN	2021RUS
		266.83	l	SEL1	-2697.20	-2521.22	0.45	DvH	2021RUS
	2-butene, (E)-	274.01	g	SEL	-2706.07	-2530.09	0.38	TN	2021RUS
		274.01	l	SEL1	-2684.77	-2508.79	0.41	DvH	2021RUS
	2-butene, (Z)-	276.87	g	SEL	-2710.16	-2534.18	0.40	TN	2021RUS
		276.87	l	SEL1	-2688.06	-2512.08	0.59	DvH	2021RUS
	isobutene	266.05	g	SEL	-2700.20	-2524.22	0.39	TN	2021RUS
		266.05	l	SEL1	-2679.60	-2503.62	0.50	DvH	2021RUS
C_5H_8	2-Methyl-1,3-butadiene	307.19	l	SEL	-3159.50	-2983.53	0.72	DvH	2021RUS
		307.19	g	SEL1	-3186.28	-3010.31	0.67	TN	2021RUS
C_5H_{10}	1-pentene	303.12	l	SEL	-3349.72	-3129.75	0.64	C	1979GOO
		303.12	g	SEL1	-3375.22	-3155.25	0.67	DvH	1979GOO
	2-methyl-1-butene	304.30	l	SEL	-3335.74	-3115.77	0.84	C	1979GOO
		304.30	g	SEL1	-3361.64	-3141.67	0.86	DvH	1979GOO
	2-pentene, (E)-	309.51	l	SEL	-3338.71	-3118.74	0.76	C	1979GOO
		309.51	g	SEL1	-3365.4	-3145.4	0.8	DvH	1979GOO
	2-pentene, (Z)-	310.09	l	SEL	-3343.21	-3123.24	0.62	C	1979GOO
		310.09	g	SEL1	-3370.0	-3150.0	0.7	DvH	1979GOO
	3-methyl-1-butene	293.21	g	SEL	-3369.00	-3149.03	0.68	DvH	1979GOO
		293.21	l	SEL1	-3345.10	-3125.13	0.62	C	1979GOO
C_6H_{12}	1-hexene	336.64	l	SEL	-4003.1	-3739.1	1.2	H2	1984MOL
		336.64	g	SEL1	-4033.7	-3769.7	1.2	DvH	1984MOL
C_7H_{14}	1-heptene	366.71	l	SEL	-4657.41	-4349.46	0.63	H2O	1984WIB
		366.71	g	SEL1	-4693.1	-4385.2	0.7	DvH	1984WIB
C_8H_{16}	1-octene	394.43	l	SEL	-5312.9	-4960.9	1.2	C	1961ROC
		394.43	g	SEL1	-5353.5	-5001.5	1.2	DvH	1961ROC
Alkadienes									
C_3H_4	allene	238.65	g	SEL	-1941.86	-1853.87	0.24	TN	2021RUS
		238.65	l	SEL1	-1925.30	-1837.31	0.69	DvH	2021RUS
C_4H_6	1,2-butadiene	284.06	g	SEL	-2593.79	-2461.81	0.46	TN	2021RUS

		284.06	l	SEL1	-2570.11	-2438.13	0.66	TN	2021RUS
	1,3-butadiene	268.44	g	SEL	-2542.28	-2410.30	0.33	TN	2021RUS
		268.44	l	SEL1	-2521.18	-2389.20	0.43	DvH	2021RUS
C_5H_8	1,2-pentadiene	318.80	l	SEL	-3222.90	-3046.92	0.69	DvH	1955FRA
		318.80	g	SEL1	-3251.60	-3075.62	0.67	C	1955FRA
	1,3-pentadiene, (E)-	315.32	l	SEL	-3158.90	-2982.92	0.78	DvH	1955FRA
		315.32	g	SEL1	-3186.70	-3010.72	0.67	C	1955FRA
	1,3-pentadiene, (Z)-	317.18	l	SEL	-3165.3	-2989.3	1.4	DvH	1955FRA
		317.18	g	SEL1	-3193.60	-3017.62	0.92	C	1955FRA
	1,4-pentadiene	299.12	g	SEL	-3217.2	-3041.2	1.3	C	1955FRA
		299.12	l	SEL1	-3192.0	-3016.0	1.3	DvH	1955FRA
Alkynes									
C_2H_2	acetylene	188.41	g	SEL	-1301.06	-1257.06	0.13	TN	2021RUS
		188.41	l	SEL1	-1293.7	-1249.7	4.4	DvH	2021RUS
C_3H_4	propyne	249.80	g	SEL	-1937.72	-1849.73	0.22	TN	2021RUS
		249.80	l	SEL1	-1918.14	-1830.15	0.56	DvH	2021RUS
C_4H_6	1-butyne	281.18	g	SEL	-2598.06	-2466.08	0.67	TN	2021RUS
		281.18	l	SEL1	-2574.36	-2442.38	0.71	DvH	2021RUS
	2-butyne	300.12	l	SEL	-2551.15	-2419.17	0.58	DvH	2021RUS
		300.12	g	SEL1	-2577.85	-2445.87	0.49	TN	2021RUS
C_5H_8	1-pentyne	313.51	l	SEL	-3226.6	-3050.6	2.3	DvH	1945WAG
		313.51	g	SEL1	-3255.0	-3079.0	2.1	E	1945WAG
	2-pentyne	329.27	l	SEL	-3208.8	-3032.8	2.2	DvH	1945WAG
		329.27	g	SEL1	-3239.6	-3063.6	2.1	E	1945WAG
C_6H_{10}	1-hexyne	344.53	l	SEL	-3879.3	-3659.4	1.6	DvH	1979ROG
		344.53	g	SEL1	-3912.3	-3692.3	1.2	H2	1979ROG
	2-hexyne	357.59	l	SEL	-3861.9	-3641.9	2.5	DvH	1979ROG
		357.59	g	SEL1	-3897.7	-3677.7	2.4	H2	1979ROG
	3-hexyne	354.58	l	SEL	-3860.2	-3640.2	1.9	DvH	1979ROG
		354.58	g	SEL1	-3895.4	-3675.4	1.9	H2	1979ROG
C_4H_4	butenyne	279.18	g	SEL	-2434.97	-2346.98	0.58	TN	2021RUS
		279.18	l	SEL1	-2411.8	-2323.8	2.1	TN	2021RUS
C_5H_6	3-penten-1-yne	317.05	l	SEL	-3050.7	-2918.7	3.6	R	2019DIK
		317.05	g	SEL1	-3078.3	-2946.3	3.3	R	2019DIK
	3-penten-1-yne, (E)-	323.65	l	SEL	-3050.7	-2918.8	3.2	R	2019DIK
		323.65	g	SEL1	-3079.1	-2947.1	2.8	R	2019DIK
	3-penten-1-yne, (Z)-	317.15	l	SEL	-3050.2	-2918.2	2.9	R	2019DIK

		317.15	g	SEL1	-3077.5	-2945.5	2.8	R	2019DIK
C_4H_2	butadiyne	283.65	g	SEL	-2319.73	-2275.74	0.58	TN	2021RUS
		283.65	l	SEL1	-2296.49	-2252.50	1.17	DvH	2021RUS
Cycloalkanes									
C_3H_6	cyclopropane	240.27	g	SEL	-2091.75	-1959.76	0.40	TN	2021RUS
		240.27	l	SEL1	-2073.63	-1941.64	0.53	TN	2021RUS
C_4H_8	cyclobutane	285.64	g	SEL	-2745.02	-2569.04	0.39	TN	2021RUS
		285.64	l	SEL1	-2721.14	-2545.16	0.40	TN	2021RUS
C_5H_{10}	cyclopentane	322.40	l	SEL	-3291.40	-3071.43	0.43	TN	2021RUS
		322.40	g	SEL1	-3320.09	-3100.12	0.43	TN	2021RUS
	methylcyclobutane	310.00	l	SEL	-3339.5	-3119.5	1.3	DvH	1950HUM
		310.00	g	SEL1	-3352.0	-3132.0	1.3	C	1950HUM
C_6H_{12}	cyclohexane	353.87	l	SEL	-3919.73	-3655.77	0.30	TN	2021RUS
		353.87	g	SEL1	-3952.87	-3688.91	0.31	TN	2021RUS
	methylcyclopentane	344.96	l	SEL	-3937.74	-3673.78	0.37	TN	2021RUS
		344.96	g	SEL1	-3969.52	-3705.56	0.38	TN	2021RUS
C_7H_{14}	methylcyclohexane	374.12	l	SEL	-4565.29	-4257.33	0.96	C	1946PRO
		374.12	g	SEL1	-4600.69	-4292.73	1.08	DvH	1946PRO
$C_{10}H_{20}$	1,3-diethylcyclohexane	445.70	l	SELu	-6515.9	-6076.0	6.2	R	2019DIK
		445.70	g	SEL1u	-6562.7	-6122.8	6.0	R	2019DIK
Cycloalkenes									
C_4H_6	cyclobutene	275.74	g	SEL	-2591.98	-2460.00	0.71	TN	2021RUS
		275.74	l	SEL1	-2569.73	-2437.75	0.74	DvH	2021RUS
C_5H_8	cyclopentene	317.39	l	SEL	-3117.56	-2941.59	0.52	TN	2021RUS
		317.39	g	SEL1	-3145.85	-2969.88	0.47	TN	2021RUS
	methylenecyclobutane	315.00	l	SEL	-3204.7	-3028.7	0.5	C	1974GOO
		315.00	g	SEL1	-3232.40	-3056.42	0.65	C	1974GOO
C_6H_{10}	cyclohexene	356.10	l	SEL	-3752.00	-3532.03	0.32	TN	2021RUS
		356.10	g	SEL1	-3785.56	-3565.59	0.33	TN	2021RUS
Bicycloalkanes									
$C_{10}H_{12}$	tetralin	480.56	l	SEL	-5621.5	-5357.6	1.0	C	1976GOO
		480.56	g	SEL1	-5676.5	-5412.6	1.4	DvH	1976GOO
$C_{10}H_{18}$	cis-decalin	468.93	l	SEL	-6287.7	-5891.8	1.3	C	1941DAV
		468.93	g	SEL1	-6337.9	-5942.0	2.5	DvH	1941DAV
	trans-decalin	460.42	l	SEL	-6278.9	-5883.0	1.3	C	1941DAV
		460.42	g	SEL1	-6327.4	-5931.5		DvH	1941DAV
$C_{12}H_{22}$	1,1'-bicyclohexyl	511.10	l	SEL	-7593.0	-7109.0	1.2	C	1976GOO

	511.10	g	SEL1	-7651.0	-7167.0	0.3	DvH	1976GOO
$C_{10}H_{12}$ tetralin	480.56	l	SEL	-5621.5	-5357.6	0.9	C	1976GOO
	480.56	g	SEL1	-5676.54	-5412.58	1.05	DvH	1976GOO

Aromatic Hydrocarbons									
C_6H_6	benzene	353.22	l	SEL	-3267.51	-3135.53	0.23	TN	2021RUS
		353.22	g	SEL1	-3301.45	-3169.47	0.23	TN	2021RUS
		278.70	s	SEL2	-3256.83	-3124.85	0.92	DfusH	2008ROU
C_7H_8	toluene	383.75	l	SEL	-3909.71	-3733.73	0.34	TN	2021RUS
		383.75	g	SEL1	-3947.7	-3771.8		TN	2021RUS
		178.20	s	SEL2	-3899.8	-3723.8	1.5	R	2008ROU
C_8H_{10}	ethylbenzene	408.96	l	SEL	-4564.41	-4344.44	0.55	TN	2021RUS
		408.96	g	SEL1	-4606.67	-4386.70	0.55	TN	2021RUS
	m-xylene	412.25	l	SEL	-4551.86	-4331.89	0.63	C	1946PRO
		412.25	g	SEL1	-4594.46	-4374.49	0.69	DvH	1946PRO
	o-xylene	417.56	l	SEL	-4552.9	-4332.9	1.0	C	1945PRO
		417.56	g	SEL1	-4596.26	-4376.29	1.04	DvH	1945PRO
	p-xylene	411.47	l	SEL	-4552.86	-4332.89	0.92	C	1946PRO
		411.47	g	SEL1	-4595.16	-4375.19	0.97	C(l)	1946PRO
C_9H_{12}	isopropylbenzene	425.54	l	SEL	-5215.44	-4951.48	0.96	C	1945PRO
		425.54	g	SEL1	-5260.54	-4996.58	1.09	DvH	1945PRO
$C_{10}H_{14}$	m-isopropyltoluene	448.35	l	SEL	-5857.3	-5549.3	1.0	C	1973GOO
		448.35	g	SEL1	-5906.9	-5598.9	1.3	DvH	1973GOO
	o-isopropyltoluene	451.50	l	SEL	-5862.62	-5554.66	0.84	C	1973GOO
		451.50	g	SEL1	-5912.26	-5604.30	1.19	DvH	1973GOO
	p-isopropyltoluene	450.27	l	SEL	-5857.9	-5549.9	1.0	C	1973GOO
		450.27	g	SEL1	-5907.28	-5599.32	1.11	DvH	1973GOO
C_8H_8	styrene	418.45	l	SEL	-4395.42	-4219.45	0.48	TN	2021RUS
		418.45	g	SEL1	-4439.45	-4263.48	0.48	TN	2021RUS
$C_{10}H_8$	naphthalene	353.65	s	SEL	-5154.7	-4978.7	3.4	R	2008ROU
		353.65	l	SEL1	-5173.0	-4997.0	1.7	DvH	2008ROU
		491.11	g	SEL2	-5228.7	-5052.7	1.5	R	2008ROU
$C_{11}H_{10}$	1-methylnaphthalene	517.84	l	SEL	-5814.0	-5594.1	1.7	C	1960SPE
		517.84	g	SEL1	-5874.1	-5654.2	1.9	DvH	1960SPE
		242.52	s	SEL2	-5807.1	-5587.1	1.7	DfusH	1960SPE
	2-methylnaphthalene	307.69	s	SEL	-5802.7	-5582.7	1.5	C	1960SPE
		514.25	l	SEL1	-5814.8	-5594.9	2.2	DfusH	1960SPE
		514.25	g	SEL2	-5860.1	-5640.2	1.8	DvH	1960SPE
C_8H_8	styrene	418.45	l	SEL	-4394.87	-4218.90	0.84	C	1945PRO
		418.45	g	SEL1	-4438.35	-4262.37	0.92	C	1945PRO

OXIDIZED HYDROCARBONS									
Carbon Oxides									
CO_2	carbon dioxide	194.69	g	SEL	0.000	0.000	0.021	TN	2021RUS
CO	carbon monoxide	81.64	g	SEL	-282.952	-282.952	0.030	TN	2021RUS
Alkanols									
CH_4O	methanol	337.63	l	SEL	-726.52	-638.53	0.16	TN	2021RUS
		337.63	g	SEL1	-764.22	-676.23	0.16	TN	2021RUS
C_2H_6O	ethanol	351.57	l	SEL	-1366.92	-1234.94	0.23	TN	2021RUS
		351.57	g	SEL1	-1409.39	-1277.41	0.23	TN	2021RUS
C_3H_8O	1-propanol	370.26	l	SEL	-2021.03	-1845.06	0.25	TN	2021RUS
		370.26	g	SEL1	-2068.49	-1892.52	0.26	TN	2021RUS
	isopropanol	355.39	l	SEL	-2004.83	-1828.86	0.36	TN	2021RUS
		355.39	g	SEL1	-2050.27	-1874.30	0.36	TN	2021RUS
$C_4H_{10}O$	1-butanol	390.77	l	SEL	-2676.18	-2456.21	0.24	C	1975MOS
		390.77	g	SEL1	-2728.68	-2508.71	0.39	DvH	1975MOS
	isobutanol	380.90	l	SEL	-2669.64	-2449.67	0.59	C	1965CHA
		380.90	g	SEL1	-2720.48	-2500.51	0.59	DvH	1965CHA
	tert-butanol	355.50	l	SEL	-2643.95	-2423.98	0.79	C	1960SKI
		355.50	g	SEL1	-2689.7	-2469.7	1.5	DvH	1960SKI
		298.87	s	SEL2	-2636.7	-2416.7	5.1	R	2019DIK
$C_5H_{12}O$	1-pentanol	410.90	l	SEL	-3330.91	-3066.95	0.28	C	1975MOS
		410.90	g	SEL1	-3387.60	-3123.63	0.35	DvH	1975MOS
	2-methyl-1-butanol	402.14	l	SEL	-3325.95	-3061.98	0.54	C	1965CHA
	isopentanol	404.73	l	SEL	-3326.2	-3062.2	0.5	C	1965CHA
		404.73	g	SEL1	-3381.2	-3117.3	1.4	DvH	1965CHA
Sugars									
$C_2H_6O_2$	1,2-ethanediol	470.73	l	SEL	-1189.19	-1057.21	0.37	TN	2021RUS
		470.73	g	SEL1	-1255.06	-1123.08	0.40	TN	2021RUS
$C_3H_8O_2$	2-methoxyethanol	397.54	l	SEL	-1901.7	-1725.7	7.6	H2O	1977GUT
		397.54	g	SEL1	-1947	-1771	8	DvH	1977GUT
$C_3H_8O_3$	glycerin	563.00	l	SEL	-1654.3	-1478.3	0.4	C	1988BAS
		563.00	g	SEL1	-1746.00	-1570.02	0.99	DvH	1988BAS
		563.00	s	SEL2	-1636.02	-1460.04	0.99	DfusH	1988BAS
$C_6H_{12}O_6$	alpha-D-glucose	415.0	s	SEL	-2805.0	-2541.0	1.3	C	1960PON
		706	g	SEL1	-2944	-2680	49	DsubH	1960PON
$C_6H_{12}O_6$	fructose	415.0	s(d)	SEL	-2810.4	-2546.4	0.3	C	1939CLA
$C_{12}H_{22}O_{11}$	sucrose	415.0	s(d)	SEL	-5643.4	-5159.5	1.8	C	1960PON

Ethers									
C_2H_6O	dimethyl ether	248.37	g	SEL	-1460.41	-1328.43	0.40	TN	2021RUS
		248.37	l	SEL1	-1441.9	-1309.9	1.1	DvH	2021RUS
C_3H_8O	ethyl methyl ether	280.59	g	SEL	-2106.41	-1930.44	0.58	DvH	2021RUS
		280.59	l	SEL1	-2082.5	-1906.5	1.2	TN	2021RUS
$C_4H_{10}O$	diethyl ether	307.56	l	SEL	-2725.25	-2505.28	0.82	TN	2021RUS
		307.56	g	SEL1	-2752.62	-2532.65	0.82	TN	2021RUS
$C_6H_{14}O$	diisopropyl ether	341.49	l	SEL	-4010.4	-3702.4	1.3	C	1965COL
		341.49	g	SEL1	-4043.1	-3735.1	1.4	DvH	1965COL
Aldehydes									
CH_2O	formaldehyde	254.13	g	SEL	-570.088	-526.094	0.096	TN	2021RUS
		254.13	l	SEL1	-549.65	-505.65	0.55	TN	2021RUS
C_2H_4O	acetaldehyde	293.56	g	SEL	-1193.06	-1105.08	0.25	TN	2021RUS
		293.56	l	SEL1	-1166.84	-1078.86	0.47	TN	2021RUS
C_3H_6O	propanal	321.19	l	SEL	-1821.20	-1689.21	0.36	TN	2021RUS
		321.19	g	SEL1	-1851.14	-1719.15	0.26	TN	2021RUS
C_4H_8O	butanal	347.95	l	SEL	-2477.72	-2301.74	0.84	TN	2021RUS
		347.95	g	SEL1	-2511.40	-2335.42	0.85	TN	2021RUS
C_3H_4O	1-propenal	264.25	g	SEL	-1687.9	-1599.9		TN	2021RUS
	2-propenal	325.40	l	SEL	-1656.4	-1568.4	1.4	TN	2021RUS
		325.40	g	SEL1	-1686.4	-1598.4	1.2	TN	2021RUS
Ketones									
C_3H_6O	acetone	329.22	l	SEL	-1789.79	-1657.80	0.35	TN	2021RUS
		329.22	g	SEL1	-1821.17	-1689.18	0.35	TN	2021RUS
C_4H_8O	butanone	352.74	l	SEL	-2443.83	-2267.85	0.79	TN	2021RUS
		352.74	g	SEL1	-2478.75	-2302.77	0.79	TN	2021RUS
Carboxylic Acids									
CH_2O_2	formic acid	374.05	l	SEL	-254.59	-210.60	0.20	TN	2021RUS
		374.05	g	SEL1	-300.92	-256.93	0.22	TN	2021RUS
		281.47	s	SEL2	-241.9	-197.9	1.0	DfusH	2021RUS
$C_2H_4O_2$	acetic acid	391.20	l	SEL	-874.95	-786.97	0.18	TN	2021RUS
		391.20	g	SEL1	-925.86	-837.88	0.38	TN	2021RUS
		289.70	s	SEL2	-863.23	-775.25	0.35	DfusH	2021RUS
C_3H_6O	propanoic acid	413.99	l	SEL	509.60	509.60	0.18	TN	2021RUS
		413.99	g	SEL1	454.24	454.24	0.28	TN	2021RUS
C_4H_8O	n-butanoic acid	436.42	l	SEL	-2183.50	-2007.53	0.59	C	1964LEB
		436.42	g	SEL1	-2241.73	-2065.76	0.43	DvH	1964LEB

Esters									
$C_3H_6O_2$	ethyl formate	327.29	l	SEL	-1611.8	-1479.8	1.2	TN	2021RUS
		327.29	g	SEL1	-1643.9	-1511.9	1.2	TN	2021RUS
$C_2H_4O_2$	methyl formate	305.14	l	SEL	-970.10	-882.12	0.86	TN	2021RUS
		305.14	g	SEL1	-998.68	-910.70	0.84	TN	2021RUS
$C_4H_8O_2$	ethyl acetate	350.21	l	SEL	-2237.35	-2061.37	0.46	H2O	1991WIB2
		350.21	g	SEL1	-2272.49	-2096.51	0.51	H2O	1991WIB2
$C_4H_6O_2$	vinyl acetate	345.33	l	SEL	-2080.6	-1948.6	2.0	H2	1980VIL
		345.33	g	SEL1	-2117.7	-1985.8	2.2	DvH	1980VIL
$C_5H_8O_2$	ethyl acrylate	372.59	l	SEL	-2740.1	-2564.1		H2	1980VIL
		372.59	g	SEL1	-2779.3	-2603.3		DvH	1980VIL
	methyl methacrylate	369.73	l	SEL	-2728.3	-2552.3	4.0		1980VIL
		369.73	g	SEL1	-2768.3	-2592.4	4.0		1980VIL
Oxacyclohydrocarbons									
C_2H_4O	oxirane	283.59	g	SEL	-1306.00	-1218.02	0.37	TN	2021RUS
		283.59	l	SEL1	-1281.07	-1193.09	0.44	TN	2021RUS
C_4H_4O	furan	304.51	l	SEL	-2083.5	-1995.5	0.6	C	1952GUT
		304.51	g	SEL1	-2111.1	-2023.1	0.6	DvH	1952GUT
$C_3H_6O_3$	1,3,5-trioxane	335.65	s	SEL	-1515.70	-1383.72	0.30	C	1969MAN
		387.20	l	SEL1	-1526.4	-1394.4	4.8	DfusH	1969MAN
		387.20	g	SEL2	-1572.3	-1440.3	0.5	DsubH	1969MAN
$C_4H_8O_2$	1,3-dioxane	378.13	l	SEL	-2339.86	-2163.88	0.99	C	1982BYS
		378.13	g	SEL1	-2378.95	-2202.97	0.99	DvH	1982BYS
	1,4-dioxane	374.25	l	SEL	-2362.23	-2186.25	0.99	C	1982BYS
		374.25	g	SEL1	-2362.28	-2186.30	0.99	DvH	1982BYS
$C_{10}H_{16}O$	D-camphor	451.8	s	SEL	-5902.0	-5550.0	3.0	C	1977STE
		493.00	g	SEL1	-5953.9	-5601.9	3.1	DsubH	1977STE
		451.8	l	SEL2	-5908.8	-5556.9	3.2	DvH	1977STE
$C_4H_2O_3$	2,5-Furandione	325.65	s	SEL	-1389.50	-1345.51	0.67	C	1964WIL
		478.33	g	SEL1	-1458.5	-1414.5	2.1	DvH	1964WIL
		478.33	l	SEL2	-1401.0	-1357.0	2.1	DfusH	1964WIL
Aromatic Alcohols									
C_6H_6O	phenol	314.15	s	SEL	-3055.98	-2924.00	0.65	TN	2021RUS
		454.91	g	SEL1	-3124.99	-2993.01	0.63	TN	2021RUS
		454.91	l	SEL2	-3071.06	-2939.08	0.70	DfusH	2021RUS
C_7H_8O	3-methylphenol	475.28	l	SEL	-3703.89	-3527.91	0.59	C	1960AND
		475.28	g	SEL1	-3765.6	-3589.6	1.2	DvH	1960AND

		285.37	s	SEL2	-3693.18	-3517.20	0.78	DfusH	1960AND
	benzyl alcohol	478.50	l	SEL	-3736.9	-3561.0	1.3	C	1954PAR
		478.50	g	SEL1	-3801.7	-3625.8	1.4	DvH	1954PAR
Oxa-Aromatics									
C_7H_6O	benzaldehyde	451.15	l	SEL	-3525.01	-3393.03	1.10	TN	2021RUS
		451.15	g	SEL1	-3574.74	-3442.76	0.91	TN	2021RUS
$C_7H_6O_2$	benzoic acid	395.50	s	SEL	-3227.01	-3095.03	0.18	TN	2021RUS
		523.53	g	SEL1	-3317.62	-3185.64	0.21	TN	2021RUS
		523.53	l	SEL2	-3238.72	-3106.74	0.21	DvH	2021RUS

NITROGEN-SUBSTITUTED HYDROCARBONS									
Hydrogen Cyanide									
CHN	hydrogen cyanide	298.79	l	SEL	-639.08	-617.08	0.30	DvH	2021RUS
		298.79	g	SEL1	-665.669	-643.672	0.092	TN	2021RUS
Alkylamines									
CH_5N	methylamine	266.84	g	SEL	-1086.81	-976.83	0.24	TN	2021RUS
		266.84	l	SEL1	-1062.79	-952.81	0.45	TN	2021RUS
C_2H_7N	ethylamine	289.79	g	SEL	-1737.31	-1583.33	0.54	TN	2021RUS
		289.79	l	SEL1	-1713.25	-1559.27	0.55	TN	2021RUS
C_3H_9N	1-propylamine	320.38	l	SEL	-2365.13	-2167.15	0.41	TN	2021RUS
		320.38	g	SEL1	-2396.55	-2198.57	0.42	TN	2021RUS
	isopropylamine	304.92	l	SEL	-2354.37	-2156.39	0.52	TN	2021RUS
		304.92	g	SEL1	-2383.08	-2185.10	0.53	TN	2021RUS
$C_4H_{11}N$	n-butylamine	350.12	l	SEL	-3018.46	-2776.50	1.13	C	1959EVA
		350.12	g	SEL1	-3054.17	-2812.21	1.13	DvH	1959EVA
C_2H_7N	dimethylamine	280.02	g	SEL	-1769.79	-1615.81	0.42	TN	2021RUS
		280.02	l	SEL1	-1743.91	-1589.93	0.37	TN	2021RUS
C_3H_9N	methylethylamine	305.60	l	SEL	-2391.4	-2193.5	2.3	TN	2021RUS
		305.60	g	SEL1	-2420.7	-2222.8	1.1	TN	2021RUS
	trimethylamine	276.00	g	SEL	-2439.91	-2241.93	0.76	TN	2021RUS
		276.00	l	SEL1	-2417.80	-2219.82	0.87	TN	2021RUS
$C_6H_{15}N$	triethylamine	361.93	l	SEL	-4377.09	-4047.14	0.54	C	1966LEB
		361.93	g	SEL1	-4412.49	-4082.54	0.59	DvH	1966LEB
$C_6H_{13}N$	cyclohexylamine	406.98	l	SEL	-4071.3	-3785.3	1.3	C	1979STE
		406.98	g	SEL1	-4113.8	-3827.9	1.3	DvH	1979STE
Alkanenitriles									
C_2H_3N	ethanenitrile	355.05	l	SEL	-1256.29	-1190.30	0.22	TN	2021RUS
		355.05	g	SEL1	-1289.74	-1223.75	0.25	TN	2021RUS
C_3H_5N	propanenitrile	370.73	l	SEL	-1910.62	-1800.64	0.54	C	1971HAL
		370.73	g	SEL1	-1946.60	-1836.62	0.62	C	1971HAL
C_4H_7N	butanenitrile	390.77	l	SEL	-2568.68	-2414.70	0.92	C	1959EVA
		390.77	g	SEL1	-2605.67	-2451.69	0.92	DvH	1959EVA
C_3H_3N	propenenitrile	351.13	l	SEL	-1756.40	-1690.41	0.42	C	1971HAL
		351.13	g	SEL1	-1789.04	-1723.05	0.72	DvH	1971HAL
Azahydrocarbons									
C_2N_2	cyanogen	252.00	g	SEL	-1097.07	-1097.07	0.41	TN	2021RUS
		252.00	l	SEL1	-1076.13	-1076.13	0.42	TN	2021RUS

$C_2H_8N_2$	1,1-dimethylhydrazine	335.57	l	SEL	-1978.7	-1802.7	3.6	C	1960DON
		335.57	g	SEL1	-2013.7	-1837.7	3.6	DvH	1960DON
$C_3H_6N_6$	1,3,5-triazine-2,4,6-triamine	618	s	SEL	-1972.0	-1840.0	3.0	C	1973SEL
C_6H_7N	aniline	457.30	l	SEL	-3393.06	-3239.08	0.84	C	1962HAT
		457.30	g	SEL1	-3448.27	-3294.30	0.88	DvH	1962HAT
$C_8H_{11}N$	*N*,*N*-dimethylaniline	466.47	l	SEL	-4767.8	-4525.8	3.2	C	1982FUR
		466.47	g	SEL1	-4820.6	-4578.7	3.2	DvH	1982FUR
		275.65	s	SEL2	-4756.2	-4514.3	3.2	DfusH	1982FUR
$C_6H_{15}NO_3$	triethanolamine	623.15	l	SEL	-3840.6	-3510.6	1.5	C	1982MIN
		623.15	g	SEL1	-3946.3	-3616.3	2.7	DvH	1982MIN
Nitroalkanes and Nitrites									
CH_3NO_3	methyl nitrate	338.00	g	SEL	-700.0	-634.1	1.3	E	1959RAY
CN_4O_8	tetranitromethane	397.95	l	SEL	-431.8	-431.8	1.7	C	1975LEB
		397.95	g	SEL1	-475.7	-475.7	1.7	DvH	1975LEB
		287.05	s	SEL2	-395.4	-395.4	4.3	DfusH	1975LEB
CH_3NO_2	nitromethane	374.34	l	SEL	-709.25	-643.25	0.43	TN	2021RUS
		374.34	g	SEL1	-747.51	-681.51	0.46	TN	2021RUS
$C_9H_6N_2O_2$	2,4-diisocyanatotoluene	524.83	l	SEL	-4235.0	-4103.1		C	1962STR
		524.83	g	SEL1	-4284.5	-4152.5		DvH	1962STR
		293.65	s	SEL2	-4168.0	-4036.0		est	1985CHR
$C_6H_5NO_2$	nitrobenzene	483.81	l	SEL	-3082.0	-2972.0	1.4	TN	2021RUS
		483.81	g	SEL1	-3137.0	-3027.0	1.4	TN	2021RUS
$C_7H_5N_3O_6$	trinitrotoluene	355.10	s	SEL	-3406.0	-3296.0	3.0	C	1976ROU
		621.00	g	SEL1	-3519.2	-3409.2	3.4	DsubH	1976ROU
		621.00	l	SEL2	-3493.0	-3383.0	3.6	DvH	1976ROU

SULFUR-SUBSTITUTED HYDROCARBONS										
Akanethiols										
CH_4S	methanethiol	279.05	g	SEL	-1544.57	-1393.24	0.51	DvH		1961GOO
		279.05	l	SEL1	-1520.8	-1083.60	0.5	R	a	1961GOO
C_2H_6S	ethanethiol	308.19	l	SEL	-2173.17	-1977.85	0.42	C	a	1957MCC
		308.19	g	SEL1	-2200.3	-1675.12	0.43	DvH		1957MCC
Sulfides										
CS_2	carbon disulfide	318.35	l	SEL	-1687.2	-1560.5	0.5	C	a	1961GOO
		318.35	g	SEL1	-1714.5		0.5	DvH		1961GOO
C_2H_6S	dimethyl sulfide	310.42	l	SEL	-2181.45	-1656.31	0.33	C	a	1957MCC
		310.42	g	SEL1	-2208.8	-1683.70	0.59	DvH		1957MCC
C_2H_6OS	dimethyl sulfoxide	463.86	l	SEL	-2037.30	-1512.16	1.25	C	g	1994MAS
		463.86	g	SEL1	-2095.9	-1570.8	1.5	DvH		1994MAS

HALOGENATED HYDROCARBONS										
Fluoroalkanes										
CH_3F	fluoromethane	194.65	g	SEL	-764.86	-672.54	0.28	TN	k	2021RUS
		194.65	l	SEL1	-756.33	-664.01	1.15	DvH		2021RUS
CH_2F_2	difluoromethane	221.50	g	SEL	-584.82	-488.16	0.40	TN	k	2021RUS
		221.50	l	SEL1	-566.84	-470.18	0.43	TN		2021RUS
CHF_3	trifluoromethane	188.75	g	SEL	-374.80	-273.81		TN	k	2021RUS
		188.75	l	SEL1	-366.34	-265.35		TN		2021RUS
CF_4	tetrafluoromethane	145.56	g	SEL	-172.55	-67.23		TN	k	2021RUS
		145.56	l	SEL1	-160.74	-55.42		DvH		2021RUS
C_2H_5F	fluoroethane	236.05	g	SEL	-1407.52	-1271.21	0.40	TN		2021RUS
		236.05	l	SEL1	-1391.21	-1254.89	0.47	DvH		2021RUS
$C_2H_4F_2$	1,1-difluoroethane	249.13	g	SEL	-1212.14	-1071.49	0.60	DvH		2021RUS
		249.13	l	SEL1	-1193.66	-1053.01	0.88	TN		2021RUS
	1,2-difluoroethane	293.00	g	SEL	-1267.04	-1126.39	0.84	TN		2021RUS
		293.00	l	SEL1	-1245.91	-1105.26	0.98	DvH		2021RUS
$C_2H_3F_3$	1,1,1-trifluoroethane	225.91	g	SEL	-1008.3	-863.4	1.7	C		1965KOL
		225.91	l	SEL1u	-988.2	-843.2	2.0	DvH		1965KOL
	1,1,2-trifluoroethane	276.81	g	SEL	-1059	-914	10	H2		1965KOL
		276.81	l	SEL1	-1035	-890	10	DvH		1965KOL
$C_2H_2F_4$	1,1,1,2-tetrafluoroethane	247.08	g	SEL	-883.7	-734.4	2.0	CBS		1988BER
		247.08	l	SEL1	-865.6	-716.3	2.0	DvH		1988BER
	1,1,2,2-tetrafluoroethane	253.23	g	SEL	-910.1	-760.8	2.0	CBS		1988BER
		253.23	l	SEL1	-890.3	-741.0	2.3	G3B3		2016GOO
C_2HF_5	pentafluoroethane	225.06	g	SEL	-701	-547	8	G3B3		2016GOO
		225.06	l	SEL1	-687	-533	8	DvH		2016GOO
C_2F_6	hexafluoroethane	194.87	g	SEL	-513.33	-355.34		TN		2021RUS
		194.87	l	SEL1	-506.33	-348.34		DvH		2021RUS
Fluoroalkenes										
$C_2H_3F_3$	fluoroethene	201.65	g	SEL	-1251.41	-1159.09	0.48	TN		2021RUS
		201.65	l	SEL1	-1240.61	-1148.29	0.90	DvH		2021RUS
$C_2H_2F_2$	1,1-difluoroethene	190.15	g	SEL	-1078.41	-981.75	0.80	TN		2021RUS
		190.15	l	SEL1	-1074.0	-977.3	2.7	DvH		2021RUS
	1,2-difluoroethene, (E)-	231.15	g	SEL	-1123.0	-1026.3	0.9	TN		2021RUS
		231.15	l	SEL1	-1108.05	-1011.39	1.39	DvH		2021RUS
	1,2-difluoroethene, (Z)-		g	SEL	-1119.4	-1022.7	0.9	TN		2021RUS
		253.15	l	SEL1	-1105.6	-1008.9	1.3	DvH		2021RUS

C_2HF_3	trifluoroethene	211.70	g	SEL	-966.2	-865.2	1.6	TN	2021RUS
		211.70	l	SEL1	-954.8	-853.8	1.9	DvH	2021RUS
C_2F_4	tetrafluoroethene	197.51	g	SEL	-825.10	-719.77	0.61	TN	2021RUS
		197.51	l	SEL1	-819.00	-713.67	1.44	DvH	2021RUS
Chloroalkenes									
CH_3Cl	chloromethane	249.00	g	SEL	-763.51	-645.24	0.39	TN	2021RUS
		249.00	l	SEL1	-743.61	-625.34	0.25	TN	2021RUS
CH_2Cl_2	dichloromethane	312.92	g	SEL	-633.00	-484.44	0.52	TN	2021RUS
		312.92	l	SEL1	-603.99	-455.43	0.54	TN	2021RUS
$CHCl_3$	trichloromethane	334.42	g	SEL	-504.94	-326.09	0.50	TN	2021RUS
		334.42	l	SEL1	-473.54	-294.69	0.51	TN	2021RUS
CCl_4	tetrachloromethane	349.65	g	SEL	-392.02	-182.89	0.43	TN	2021RUS
		349.65	l	SEL1	-359.52	-150.39	0.43	TN	2021RUS
C_2H_5Cl	chloroethane	285.40	g	SEL	-1413.57	-1251.30	0.26	TN	2021RUS
		285.40	l	SEL1	-1389.14	-1226.87	0.40	TN	2021RUS
$C_2H_4Cl_2$	1,1-dichloroethane	330.42	g	SEL	-1272.61	-1080.06	0.44	TN	2021RUS
		330.42	l	SEL1	-1241.81	-1049.26	0.48	TN	2021RUS
	1,2-dichloroethane	356.70	l	SEL	-1238.5	-1045.9	3.5	R	2002MAN
		356.70	g	SEL1	-1273.7	-1081.1	3.5	R	2002MAN
$C_2H_3Cl_3$	1,1,1-trichloroethane	347.22	l	SEL	-1109.1	-886.3	2.0	R	2002MAN
		347.22	g	SEL1	-1141.7	-918.9	2.0	R	2002MAN
	1,1,2-trichloroethane	386.78	l	SEL	-1098.0	-875.2	4.0	R	2002MAN
		386.78	g	SEL1	-1138.3	-915.5	4.0	R	2002MAN
$C_2H_2Cl_4$	1,1,1,2-tetrachloroethane	403.33	l	SEL	-973.5	-720.4	2.3	R	2002MAN
		403.33	g	SEL1	-1014.6	-761.5	2.4	R	2002MAN
	1,1,2,2-tetrachloroethane	419.25	l	SEL	-964.5	-711.4	3.5	R	2002MAN
		419.25	g	SEL1	-1010.2	-757.1	3.5	R	2002MAN
C_2HCl_5	pentachloroethane	433.45	l	SEL	-844.3	-560.9	4.0	R	2002MAN
		433.45	g	SEL1	-891.7	-608.3	4.3	R	2002MAN
C_2Cl_6	hexachloroethane	462.96	l	SEL	-711.7	-398.0	2.8	TN	2021RUS
		462.96	g	SEL1	-778.8	-465.1	1.3	TN	2021RUS
Chloroalkenes									
C_2H_3Cl	chloroethene	259.35	l	SEL	-1241.13	-1122.86	0.36	TN	2021RUS
		259.35	g	SEL1	-1260.93	-1142.66	0.30	TN	2021RUS
$C_2H_2Cl_2$	1,1-dichloroethene	304.71	l	SEL	-1122.81	-974.25	0.49	TN	2021RUS
		304.71	g	SEL1	-1096.06	-947.50	0.50	TN	2021RUS
	1,2-dichloroethene, (E)-	320.73	l	SEL	-1119.74	-971.18	0.54	DvH	2021RUS

		320.73	g	SEL1	-1149.24	-1000.68	1.14	TN	2021RUS
	1,2-dichloroethene, (Z)-	333.58	l	SEL	-1086.23	-937.67	1.14	TN	2021RUS
		333.58	g	SEL1	-1117.33	-968.77	0.54	TN	2021RUS
C_2HCl_3	trichloroethene	360.50	l	SEL	-985.9	-807.0	1.5	TN	2021RUS
		360.50	g	SEL1	-951.3	-772.4	1.5	TN	2021RUS
C_2Cl_4	tetrachloroethene	394.29	l	SEL	-818.2	-609.1	1.1	TN	2021RUS
		394.29	g	SEL1	-857.9	-648.8	1.1	TN	2021RUS
Chloroalkynes									
C_2HCl	chloroethyne	243.6	g	SEL	-1182.39	-1108.12	0.70	TN	2021RUS
		243.6	l	SEL1	-1162.4	-1088.1	1.2	DvH	2021RUS
Bromoalkanes									
CH_3Br	bromomethane	276.70	g	SEL	-763.80	-635.15	0.26	TN	2021RUS
		276.70	l	SEL1	-740.47	-611.82	0.27	TN	2021RUS
CH_2Br_2	dibromomethane	370.10	l	SEL	-601.3	-432.0	1.1	TN	2021RUS
		370.10	g	SEL1	-638.3	-469.0	1.1	TN	2021RUS
$CHBr_3$	tribromomethane	422.36	l	SEL	-471.5	-261.5	1.3	TN	2021RUS
		422.36	g	SEL1	-517.6	-307.6	1.3	TN	2021RUS
CBr_4	tetrabromomethane	462.55	l	SEL	-351.6	-100.9	1.4	TN	2021RUS
		462.55	g	SEL1	-406.1	-155.4	1.3	TN	2021RUS
C_2H_5Br	bromoethane	311.54	l	SEL	-1387.66	-1215.02	0.26	TN	2021RUS
		311.54	g	SEL1	-1415.65	-1243.01	0.25	TN	2021RUS
Bromoethenes									
C_2H_3Br	bromoethene	288.60	g	SEL	-1266.79	-1138.13	0.57	TN	2021RUS
		288.60	l	SEL1	-1233.0	-1104.4	1.8	DvH	2021RUS
Chlorofluoroalkanes									
CH_2ClF	chlorofluoromethane	264.00	g	SEL	-617.7	-495.1	1.1	TN	2021RUS
		264.00	l	SEL1	-599.1	-476.5	1.5	DvH	2021RUS
$CHClF_2$	chlorodifluoromethane	232.35	g	SEL	-433.99	-307.05	1.01	TN	2021RUS
		232.35	l	SEL1	-418.29	-291.35	1.05	DvH	2021RUS
$CHCl_2F$	dichlorofluoromethane	282.05	g	SEL	-478.01	-325.12	0.92	TN	2021RUS
		282.05	l	SEL1	-454.4	-301.5	1.5	DvH	2021RUS
$CClF_3$	chlorotrifluoromethane	191.75	g	SEL	-241.78	-110.50	0.63	TN	2021RUS
		191.75	l	SEL1	-225.28	-94.00	0.70	TN	2021RUS
CCl_2F_2	dichlorodifluoromethane	243.35	g	SEL	-303.18	-145.95	0.71	TN	2021RUS
		243.35	l	SEL1	-286.38	-129.15	0.73	DvH	2021RUS
CCl_3F	trichlorofluoromethane	296.95	g	SEL	-353.80	-170.62	0.80	TN	2021RUS
		296.95	l	SEL1	-329.01	-145.83	0.81	TN	2021RUS

C_2ClF_3	chlorotrifluoroethene	244.80	g	SEL	-833.2	-701.9	2.8	DvH	1982ERA
		244.80	l	SEL1	-816.0	-684.7	2.8	C	1982ERA
Bromofluoroalkanes									
CH_2BrF	bromofluoromethane	310.00	l	SEL	-591.3	-458.3	5.2	DvH	2021RUS
		310.00	g	SEL1	-622.7	-489.7	4.9	TN	2021RUS
$CHBrF_2$	bromodifluoromethane	258.65	g	SEL	-445.5	-308.2	1.2	TN	2021RUS
		258.65	l	SEL1	-425.5	-288.2	1.6	DvH	2021RUS
$CHBr_2F$	dibromofluoromethane	338.05	l	SEL	-456.9	-283.2	5.2	DvH	2021RUS
		338.05	g	SEL1	-489.6	-316.0	4.9	TN	2021RUS
$CBrF_3$	bromotrifluoromethane	215.35	g	SEL	-254.08	-112.43	0.52	TN	2021RUS
		215.35	l	SEL1	-242.31	-100.65	0.53	TN	2021RUS
CBr_2F_2	dibromodifluoromethane	297.65	g	SEL	-322.1	-144.2	1.3	TN	2021RUS
		297.65	l	SEL1	-297.7	-119.7	1.3	DvH	2021RUS
CBr_3F	tribromofluoromethane	379.65	l	SEL	-324.4	-110.0	3.0	DvH	2021RUS
		379.65	g	SEL1	-373.7	-159.4	1.5	TN	2021RUS
Bromochloroalkanes									
CH_2BrCl	bromochloromethane	341.21	l	SEL	-605.1	-446.2	1.3	DvH	2021RUS
		341.21	g	SEL1	-637.8	-478.9	1.3	TN	2021RUS
$CHBrCl_2$	bromodichloromethane	362.65	l	SEL	-476.6	-287.3	2.2	DvH	2021RUS
		362.65	g	SEL1	-511.6	-322.3	1.2	TN	2021RUS
$CHBr_2Cl$	dibromochloromethane	393.00	l	SEL	-470.4	-270.8	4.1	DvH	2021RUS
		393.00	g	SEL1	-514.3	-314.7	3.4	TN	2021RUS
$CBrCl_3$	bromotrichloromethane	376.65	l	SEL	-363.8	-144.3	1.6	DvH	2021RUS
		376.65	g	SEL1	-399.40	-179.89	0.59	TN	2021RUS
CBr_2Cl_2	dibromodichloromethane	423.35	l	SEL	-360.5	-130.6	4.2	DvH	2021RUS
		423.35	g	SEL1	-400.0	-170.2	1.3	TN	2021RUS
CBr_3Cl	tribromochloromethane	433.00	l	SEL	-355.0	-114.7	2.9	DvH	2021RUS
		433.00	g	SEL1	-403.0	-162.7	1.5	TN	2021RUS
Bromochlorofluoroalkanes									
CHBrClF	bromochlorofluoromethane	312.60	l	SEL	-456.7	-293.5	5.1	DvH	2021RUS
		312.60	g	SEL1	-484.4	-321.1	4.9	TN	2021RUS
$CBrClF_2$	bromochlorodifluoromethane	270.65	g	SEL	-310.6	-143.0	4.9	TN	2021RUS
		270.65	l	SEL1	-289.9	-122.3	4.9	DvH	2021RUS
$CBrCl_2F$	bromodichlorofluoromethane	325.15	l	SEL	-326.8	-133.2	5.2	DvH	2021RUS
		325.15	g	SEL1	-357.6	-164.0	4.9	TN	2021RUS
CBr_2ClF	dibromochlorofluoromethane	352.65	l	SEL	-327.2	-123.3	5.2	DvH	2021RUS
		352.65	g	SEL1	-362.7	-158.8	4.9	TN	2021RUS

Carbonyl Halides									
CCl_2O	phosgene	280.71	g	SEL	-221.41	-116.85	0.27	TN	2021RUS
		280.71	l	SEL1	-198.58	-94.01	0.47	DvH	2021RUS
Pentachlorophenol									
C_6HCl_5O	pentachlorophenol	463.84	s	SEL	-2329.0	-2045.6	2.9	C	1958SIN
		582.50	l	SEL1	-2346.1	-2062.7	3.0	DsubH	1958SIN
		582.50	g	SEL2	-2420.6	-2137.2	3.0	DvH	1958SIN

4.5. References for Heats of Combustion, Formation, and Transition

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5. Heat Capacities

5.1. Overview

In this work, we compiled, evaluated, and recommended gas-phase C_p(g), liquid-phase C_p(l), and solid-phase C_p(s) heat capacities at standard state (T = 298.15 K) for hydrocarbons, substituted hydrocarbons, and a few other compounds of physical, chemical, and engineering interest. We provide about 650 values for heat capacities for about 310 compounds from about 90 source references. The substituted hydrocarbons include different classes of oxygen-, nitrogen-, sulfur-, and halogen-substituted hydrocarbons. The compounds are organized by compound class – for example, Hydrocarbons: Alkanes, Alkenes; Oxidized Hydrocarbons: Alkanols, Aldehydes; etc. The values were taken from the literature and the NIST Chemistry Webbook.[2021LIN] We checked these values against those provided in the NIST TRC Thermodata Engine (TDE) [2021DIK], and where not readily available in the literature, we utilized values from TDE. The full references are given in Section 5.4.

We provide uncertainties from the original where they were readily available. For many of the uncertainties reported in the literature, they are standard uncertainties of 1σ. For our recommended values, we provide expanded uncertainties U. In cases where uncertainties in heat capacities which were not provided (or recorded), we utilized expanded uncertainties (2σ) of 3 % for gas- and liquid-phase heat capacities, and 0.5 % for solid-phase heat capacities. These estimated expanded uncertainties were chosen based on our analysis of the cases where uncertainties were available. We found for gas-phase heat capacities that about 40% of the uncertainties were less than 1 %, about 30 % were (1 to 3) %, and about 30 % were (3 to 7) %. For liquid-phase heat capacities, we found that about 60 % were under 1 %, 15 % were (1 to 3) %, and 25 % were (3 to 6) %. For solid-phase heat capacities, we found that about 70 % were under 0.5 %, and about 30 % were (0.5 to 1.2) %. Uncertainties of 1.0 % for gas-phase heat capacities C_p(g) from TDE are generic estimates from TDE where experimental values were not available.

In the Table 5-1, heat capacities in the gas-, liquid-, and solid-phases are given by C_p(g), C_p(l), and C_p(s), respectively. The heat capacities are all at T = 298.15 K. The gas-phase heat capacities are for ideal gases at standard state, while the liquid-phase heat capacities are at saturation pressures, and the solid-phase heat capacities are either at saturation pressures or at 1 atm (101.325 kPa). For ice, H_2O(s), the solid-phase heat capacity is at the melting point 273.15 K. The column “SEL” indicates all the selected value for all phases SEL, gas-phase SEL(g), liquid-phase SEL(l), or solid-phase SEL(s) heat capacities are from the indicated source, while those labeled SEL(g), SEL(l), or SEL(s) are from the indicated source. Table 5-1 provides all of the data along with reference sources, while Table 5-2 just provides the recommended values.

5.2. **Heat Capacities (Compiled)**

This Table 5-2 contains all the heat capacities that were compiled, while the next Table 5-3 provides only the selected recommended values for heat capacities in the gas, liquid, and solid phases.

Table 5-2. Heat capacities in gas, liquid, and solid phases

Formula	Compound	SEL	C_p(g)	$u(C_p$g)	C_p(l)	$u(C_p$l)	C_p(s)	$u(C_p$s)	Reference
			J mol^{-1} K^{-1}						
Hydrogen/Oxygen									
H_2	hydrogen	SEL	28.84	0.10					1998CHA
			28.83	0.29					2019DIK
			28.68	0.06					1979BER
O_2	oxygen	SEL	29.39	0.10					1998CHA
			29.37	0.29					2019DIK
H_2O	water	SEL	33.59	0.07	75.33	0.01			2018LEM
		SEL(s)					37.77	0.38	2006FEI
			33.58	0.340	75.3	0.5	39.80	1.30	2019DIK
					75.23	0.08			1939OSB
							37.85		1936GIA
H_2O_2	hydrogen peroxide	SEL(g)	43.07						1998CHA
		SEL(s)	42.36	0.42			59.10	0.20	2019DIK
Nitrogen/Hydrogen/Oxygen									
N_2	nitrogen	SEL	29.09	0.12					1995ESP
			29.12	0.29					2019DIK
			29.12						1998CHA
			29.11	0.02					1992EWI
H_3N	ammonia	SEL(g)	35.64	0.04					2014SOU
		SEL(l)	35.54	0.36	81.4	0.8			2018LEM
			35.65	0.36	80.7	0.7			2019DIK
			35.64	0.20					1998CHA
H_4N_2	hydrazine	SEL	50.81	0.20	98.81	0.02			1998CHA
			49.14	0.49	98.67	0.39			2019DIK
HN_3	hydrogen azide	SEL	44.22	0.35					1989GUR

			44.16	0.44					2019DIK
N_2O	nitrous oxide	SEL	38.60	0.20					1998CHA
			38.54	0.39					2019DIK
ClH_4NO_4	ammonium perchlorate	SEL					128.07	0.33	1969WES
Sulfur/Hydrogen									
H_2S	hydrogen sulfide	SEL(g)	34.20	0.20					1998CHA
		SEL(l)	34.12	0.34	75.8	3.2			2019DIK
Boron/Hydrogen									
B_2H_6	diborane	SEL	58.07						1998CHA
Carbons									
C	carbon (gas)	SEL	20.79	0.00					definition
			20.88	0.21					2019DIK
			20.82	0.20					1998CHA
	graphite	SEL					8.43	0.10	1980TAY
							8.52	0.01	2019DIK
							8.62		1973BUT
Alkanes									
CH_4	methane	SEL	35.69	0.20					1989GUR
			35.66	0.36					2019DIK
C_2H_6	ethane	SEL(g)	52.49	0.20					1989GUR
		SEL(l)	52.50	0.53	160.6	1.9			2019DIK
C_3H_8	propane	SEL(g)	73.60	0.20					1973CHA
		SEL(l)	73.62	0.74	117.41	0.86			2019DIK
			72.67	0.07					1940KIS
C_4H_{10}	isobutane	SEL(g)	96.65	0.20					1975CHE
		SEL(l)	96.69	0.97	140.69	0.29			2019DIK
	n-butane	SEL(g)	98.49	0.20					1975CHE
		SEL(l)	98.57	0.99	140.50	0.87			2019DIK
C_5H_{12}	isopentane	SEL(g)	118.90	0.40					1974SCO
		SEL(l)	118.89	1.19	164.84	0.73			2019DIK
	neopentane	SEL(g)	120.83	0.25					1974SCO
		SEL(l)	120.93	1.21	169.2	6.3			2019DIK
	n-pentane	SEL(g)	120.00	0.10					1974SCO
		SEL(l)			167.19				1967MES
			120.10	1.20	167.14	0.53			2019DIK
C_6H_{14}	2,3-dimethylbutane	SEL(g)	139.40	0.70					1974SCO
		SEL(l)			189.02				1989OHN

			139.39	1.39	189.23	0.46	2019DIK
	3-methylpentane	SEL(g)	140.10	0.40			1974SCO
		SEL(l)			191.16		1989OHN
			140.11	1.40	190.67	0.35	2019DIK
	Isohexane	SEL(g)	142.2	0.2			1974SCO
		SEL(l)			193.88		1989OHN
			142.21	1.42	193.88	0.69	2019DIK
	neohexane	SEL(g)	141.5	0.30			1974SCO
		SEL(l)			189.67		1989OHN
			141.47	1.41	189.31	0.55	2019DIK
	n-hexane	SEL(g)	142.6	0.20			1974SCO
		SEL(l)			195.52		1989OHN
			142.60	1.43	196.12	0.49	2019DIK
C_7H_{16}	isoheptane	SEL(g)	164.50	0.20			1974SCO
		SEL(l)			222.92	0.45	1961HUF
			164.49	1.64	222.77	0.46	2019DIK
	neoheptane	SEL(g)	166.70	0.40			1974SCO
		SEL(l)			221.12	0.42	1961HUF
			166.74	1.67	221.13	0.53	2019DIK
	n-heptane	SEL(g)	165.20	0.30			1974SCO
		SEL(l)			224.73	0.12	1988SHI
					224.64		1988AND
			165.19	1.65	224.82	0.26	2019DIK
C_8H_{18}	2,2,4-trimethylpentane	SEL(g)	188.40	0.40			1974SCO
		SEL(l)			238.87	1.1	1976FOR
			188.40	1.88	239.12	1.21	2019DIK
	2-methylheptane	SEL(g)	187.2	0.2			1974SCO
		SEL(l)			252.0	0.4	1971MES
			187.21	1.87	251.98	0.25	2019DIK
	n-octane	SEL(g)	187.8	0.4			1987SCO
		SEL(l)			254.18	1.0	1985LAI2
			187.75	1.88	254.30	0.65	2019DIK
C_9H_{20}	*n*-nonane	SEL(g)	210.4	0.5			1974SCO
		SEL(l)			284.39	0.5	1954FIN
			210.4	2.1	283.73	1.30	2019DIK
$C_{10}H_{22}$	*n*-decane	SEL(g)	233.1	0.6	314.23	0.43	1974SCO
		SEL(l)			314.2	1.4	1984ROU

			233.0	2.3	314.23	0.43	2019DIK
$C_{16}H_{34}$	*n*-hexadecane	SEL(g)	369.2	3.7	501.14	0.70	2019DIK
		SEL(l)			499.7	1.0	1981GRO
Alkenes							
C_2H_4	ethane	SEL	43.29	0.30			1941BUR
			42.88	0.43			2019DIK
C_3H_6	propene	SEL(g)	63.79	0.13			1974BIE
		SEL(l)			102.00		1983CHA
			64.36	0.64	100.82	1.42	2019DIK
C_4H_8	1-butene	SEL(g)	85.65	0.86	128.71	0.50	2019DIK
		SEL(l)			128.96	0.40	1991TAK
					118.00		1983CHA
	2-butene, (*E*)-	SEL(g)	87.78	0.40			1940KIS2
		SEL(l)	87.74	0.88	130.0	2.2	2019DIK
	2-butene, (*Z*)-	SEL(g)	81.13	0.16	126.15	0.50	1944SCO
		SEL(l)			127.00	0.50	1983CHA
			80.21	0.80	127.01	1.18	2019DIK
	isobutene	SEL	88.13	0.88	133.6	4.2	2019DIK
C_5H_{10}	1-pentene	SEL(g)	108.16	1.08	155.04	0.51	2019DIK
		SEL(l)			154.87	0.30	1990MES
					154.00		1983CHA
	2-methyl-1-butene	SEL(g)	109.98	1.10	157.41	0.76	2019DIK
		SEL(l)			157.3	0.8	1983CHA
	2-methyl-2-butene	SEL(g)	104.99	1.05	152.65	0.73	2019DIK
		SEL(l)			152.80		1983CHA
	2-pentene, (*E*)-	SEL	108.89	1.09	156.97	0.63	2019DIK
	2-pentene, (*Z*)-	SEL	98.79	0.99	151.58	0.65	2019DIK
	3-methyl-1-butene	SEL	114.48	1.14	156.16	0.68	2019DIK
C_6H_{12}	1-hexene	SEL	130.82	1.31	183.08	0.55	2019DIK
C_7H_{14}	1-heptene	SEL	153.46	1.53	211.86	0.49	2019DIK
C_8H_{16}	1-octene	SEL	176.17	1.76	241.30	0.43	2019DIK
Alkadienes							
C_3H_4	allene	SEL(g)	59.07	0.24			1940KIS
		SEL(l)	59.06	0.59	102.0	3.7	2019DIK
C_4H_6	1,2-butadiene	SEL	79.50	0.80	123.83	0.86	2019DIK
	1,3-butadiene	SEL	79.64	0.80	123.66	0.48	2019DIK
C_5H_8	1,2-pentadiene	SEL	100.98	1.01	150.84	1.25	2019DIK

	1,3-pentadiene	SEL	98.9	6.3	148.6	4.9	2019DIK
	1,4-pentadiene	SEL	98.34	0.98	146.99	1.23	2019DIK
	2-methyl-1,3-butadiene	SEL	102.76	1.03	150.85	1.37	2019DIK
Alkynes							
C_2H_2	acetylene	SEL	44.04	0.30			1989GUR
			43.99	0.44			2019DIK
C_3H_4	propyne	SEL	60.7	0.6	92.5	5	2018LEM
			60.79				1940KIS
			60.75	0.61	109.4	4.1	2019DIK
C_4H_6	1-butyne	SEL	81.4	0.8	135.2	1.1	2019DIK
C_4H_6	2-butyne	SEL	78.1	0.8	125.3	1.3	2019DIK
C_4H_6	2-butyne				125.1		1941YOS
C_5H_8	1-pentyne	SEL	102.67	1.03	143.3	4.0	2019DIK
	2-pentyne	SEL	99.72	1.00	129.6	3.5	2019DIK
C_6H_{10}	1-hexyne	SEL	128.94	1.29	184.8	5.1	2019DIK
	2-hexyne	SEL	119.65		170.8	4.8	2019DIK
	3-hexyne	SEL	119.51	1.20	179.3	5.0	2019DIK
C_4H_4	butenyne	SEL(g)	73.18	1.0			1949STA
		SEL(l)	73.20	0.73	118.4	3.9	2019DIK
C_5H_6	3-penten-1-yne	SEL	96.3	5.9	139.5	4.7	2019DIK
C_4H_2	butadiyne	SEL(g)	73.70	1.00			1991DOR
		SEL(l)	73.66	0.74	117.0	3.6	2019DIK
Cycloalkanes							
C_3H_6	cyclopropane	SEL(g)	55.60	1.00			1986DOR2
		SEL(l)	55.58	0.56	96.37	1.42	2019DIK
			55.91				1940KIS
C_4H_8	cyclobutane	SEL(g)	70.60	1.50			1986DOR2
		SEL(l)	70.66	0.71	109.89	0.75	2019DIK
C_5H_{10}	cyclopentane	SEL(g)	82.80	2.00			1986DOR2
		SEL(l)			126.74	0.2	1985TAN
					126.87		1946DOU
			83.01	0.83	127.33	0.66	2019DIK
	methylcyclobutane	SEL	98.79	0.99	145.7	4.9	2019DIK
C_6H_{12}	cyclohexane	SEL(g)	105.30	2.00			1986DOR2
		SEL(l)			156.90		1989LAI
			106.33	1.06	156.20	0.38	2019DIK
	methylcyclopentane	SEL(g)	109.79	1.0			1960SCO

		SEL(l)			158.67	0.2	1946DOU
			109.51	1.10	158.81	0.65	2019DIK
C_7H_{14}	methylcyclohexane	SEL(g)	136.13	1.36	184.75	0.46	2019DIK
		SEL(l)			184.96	0.3	1985TAN
			136.14	1.36	185.44	1.95	2018LEM
					184.2		1946DOU
$C_{10}H_{20}$	1,3-diethylcyclohexane	SEL	204	13	270	11	2019DIK
Cyclopropanes							
C_3H_4	cyclopropene	SEL(g)	52.90	1.00			1986DOR2
		SEL(l)	52.88	0.53	95.8	3.7	2019DIK
C_4H_6	cyclobutene	SEL(g)	64.40	2.00			1986DOR2
		SEL(l)	64.45	0.64	101.0	3.4	2019DIK
C_5H_8	cyclopentene	SEL(g)	81.3	2.00			1986DOR2
		SEL(l)			122.38		1948HUF
			81.38	0.81	122.60	0.64	2019DIK
	methylenecyclobutane	SEL	87.36	0.87	131.56	0.46	2019DIK
C_6H_{10}	cyclohexene	SEL(g)	101.5	3.0			1986DOR2
		SEL(l)			148.80		1991STE
			101.58	1.02	150.66	0.83	2019DIK
					149.16		1948HUF
Cycloalkadienes							
C_4H_4	cyclobutadiene	SEL(g)	61.0	2.5			1986DOR2
		SEL(l)	60.78	0.61	112.1	3.7	2019DIK
C_5H_6	cyclopentadiene	SEL(g)	75.4	2.00			1986DOR2
		SEL(l)	75.41	0.75	119.9	3.4	2019DIK
C_6H_8	1,3-cyclohexadiene	SEL(g)	94.2	2.5			1986DOR2
		SEL(l)	94.73	0.95	143.7	2.4	2019DIK
	1,4-cyclohexadiene	SEL(g)	94.1	3.0			1986DOR2
		SEL(l)	95.03	0.95	145.6	2.6	2019DIK
Bicycloalkanes							
$C_{10}H_{18}$	*cis*-decalin	SEL(g)	168.60	1.00			1988DOR
		SEL(l)			229.17		1989OHN
	trans-decalin	SEL(g)	168.57	1.69	228.52	0.40	2019DIK
		SEL(l)			232.08		1989OHN
$C_{12}H_{22}$	cyclohexylcyclohexane	SEL(g)	218	15	286.96	0.19	2019DIK
		SEL(l)			286.92	0.2	1998CHI
Alkyl Benzenes							

C_6H_6	benzene	SEL(g)	82.2	0.20			2014RUZ
		SEL(l)			135.69	0.30	1993GRO
			82.54	0.83	135.62	0.80	2019DIK
			81.54	0.41	135.43	0.67	2018LEM
					135.71		1985TAN
					135.23		1955STA
C_7H_8	toluene	SEL(g)	103.7	0.40			1985DRA
		SEL(l)			157.09	0.30	1993GRO
			103.80	0.52	157.25	0.32	2019DIK
			103.79	0.52	156.75	0.39	2018LEM
C_8H_{10}	1,2-dimethylbenzene	SEL(g)	132.5	0.40			1985DRA
		SEL(l)			187.65	0.3	1979FOR
			132.43	0.33	187.79	0.28	2019DIK
			131.34	0.33	187.36	0.24	2018LEM
	1,3-dimethylbenzene	SEL(g)	125.80	0.40			1985DRA
		SEL(l)			184.63		1993GRO
			125.57	0.32	181.69	0.23	2018LEM
			125.89	0.63	181.68	0.32	2019DIK
					181.55		1979FOR
	1,4-dimethylbenzene	SEL(g)	125.6	0.40			1985DRA
		SEL(l)			181.94	0.3	1979FOR
			126.21	0.32	182.15	0.40	2019DIK
			126.23	0.32	182.26	0.45	2018LEM
			126.5	0.5	183.6	0.4	1943PIT
	ethylbenzene	SEL(g)	127.5	0.2			1978MIL
		SEL(l)			185.87	0.20	1997CHI
					185.57	0.3	1979FOR
			127.54	0.32	185.77	0.17	2019DIK
			127.53	0.32	185.35	0.46	2018LEM
C_9H_{12}	isopropylbenzene	SEL	159.75	1.60	215.21	0.52	2019DIK
$C_{10}H_{14}$	2-isopropyltoluene	SEL	180	12	251.4	8.3	2019DIK
	3-isopropyltoluene	SEL	180	12	250.4	8.0	2019DIK
	4-isopropyltoluene	SEL	180	12	238.5	2.8	2019DIK
Alkenyl Benzenes							
C_8H_8	ethenylbenzene	SEL(g)	120.27	1.20	181.3	2.1	2019DIK
		SEL(l)			182.60		1961WAR
Benzocycloalkanes							

C_9H_{10}	benzocyclopentane	SEL(g)	130.7	1.00					1986DOR
		SEL(l)	130.73	1.31	189.66	0.21			2019DIK
$C_{10}H_{12}$	benzocyclohexane	SEL(g)	150.9	2.00					1988DOR
		SEL(l)			217.44				1957MCC
			152.48	1.52	217.43	0.54			2019DIK
Naphthalenes									
$C_{10}H_8$	naphthalene	SEL(g)	131.94	1.32			165.69	0.46	2019DIK
		SEL(l)			196.06				1993CHI
		SEL(s)					165.69	0.5	1957MCC
$C_{11}H_{10}$	1-methylnaphthalene	SEL(g)	159.59	1.60	224.34	0.65			2019DIK
		SEL(l)			224.39				1957MCC
	2-methylnaphthalene	SEL(g)	159.83	1.60					2019DIK
		SEL(l)			195.98	0.6			1957MCC
Polycyclic Aromatic									
$C_{12}H_8$	acenaphthylene	SEL(g)	154.80	1.00					1986DOR
		SEL(s)	154.79	1.55			183	15	2019DIK
	biphenylene	SEL	159.35	1.59					2019DIK
$C_{12}H_{10}$	acenaphthene	SEL(g)	162.20	1.00					1986DOR
		SEL(s)					190.37	0.50	1977FIN
			162.17	1.62			190.38	0.45	2019DIK
$C_{13}H_{10}$	fluorene	SEL(g)	173.10	1.00					1989DOR
		SEL(s)					203.13		1977FIN
			173.12	1.73			203.14	0.50	2019DIK
$C_{14}H_8$	pyraccclene	SEL	172.50	1.50					1986DOR
			172.56	1.73					2019DIK
$C_{14}H_{10}$	anthracene	SEL(g)	184.70	1.00					1988DOR
		SEL(s)					211.70	1.00	1980RAD
			184.78	1.85			210.50	0.32	2019DIK
	phenanthrene	SEL(g)	185.70	1.86			220.63	0.54	2019DIK
		SEL(s)					220.62		1977FIN
$C_{14}H_{12}$	pyracene	SEL	187.20	1.50					1986DOR
			187.22	1.87					2019DIK
$C_{16}H_{10}$	aceanthrylene	SEL(g)	203.00	1.50					1986DOR
		SEL(l)	203.0	2.0	334	18			2019DIK
	fluoranthene	SEL(g)	203.60	2.00					1989DOR
		SEL(s)					230.25		1971WON
			206.3	2.1			230.25	0.35	2019DIK

	pyrene	SEL(g)	204.20					1988DOR
		SEL(s)				229.36		1980SMI
			201.6	2.0		229.64	0.34	2019DIK
						229.70		1971WON
$C_{18}H_{12}$	naphthacene	SEL(g)	233.40	1.50				1988DOR
		SEL(s)				236.60		1980WON
			233.1	2.3		259.37	3.09	2019DIK
	triphenylene	SEL(g)	222.1	2.2		259.20	0.33	2019DIK
		SEL(s)				229.70		1971WON
$C_{20}H_{12}$	perylene	SEL(g)	255.4	2.4				1988DOR
		SEL(s)	na			274.93	0.46	1980WON
$C_{24}H_{12}$	coronene	SEL(g)	286.6	5.0				1988DOR
		SEL(s)				313.80	1.00	1980WON
			277.9	2.8		313.81	1.21	2019DIK
Carbon Oxides								
CO	carbon monoxide	SEL	29.14	0.15				1998CHA
CO_2	carbon dioxide	SEL	37.14	0.16	284.63	1.06		2018LEM
			37.12	0.16				2019DIK
			37.12	0.20				1998CHA
			37.40	1.47				1964SEN
			37.44	0.42				1955HIL
Alkanols								
CH_4O	methanol	SEL(g)	44.04	0.03				1986CHA
		SEL(l)			81.08	0.20		1985WIL
			44.08	0.44	81.16	0.26		2019DIK
			44.0	0.4	81.3	0.8		2018LEM
					80.35			1988OKA
					80.24			1988AND
					81.56	0.4		1986TAN
C_2H_6O	ethanol	SEL(g)	65.20	0.14				1986CHA
		SEL(l)			112.25	0.30		1985WIL
			65.30	0.65	112.35	0.47		2019DIK
			65.2	0.7	112.2	1.1		2018LEM
					111.53			1988AND
					112.68			1986TAN
C_3H_8O	1-propanol	SEL(g)	85.56	0.14				1986CHA
		SEL(l)			143.74	0.4		1985WIL

					143.96	0.30			1986TAN
			85.77	0.86	143.74	0.23			2019DIK
	isopropanol	SEL(g)	89.32	0.15					1986CHA
		SEL(l)			155.0	0.3			1985WIL
			89.51	0.90	154.92	0.34			2019DIK
$C_4H_{10}O$	1-butanol	SEL(g)	108.03	0.25					1986CHA
		SEL(l)			177.06	0.35			1985WIL
					176.67	0.50			1986GAT
			108.35	1.08	177.17	0.62			2019DIK
					176.86				1988AND
					176.69				1986TAN
	2-butanol	SEL(g)	112.74	0.17					1986CHA
		SEL(l)			196.89	0.25			1985WIL
					198.03				1988OKA
			112.95	1.13	196.81	0.84			2019DIK
	isobutanol	SEL(g)	113	7	181.20	0.28			2019DIK
		SEL(l)			181.16	0.4			1985WIL
					181.05				1988OKA
	tert-butanol	SEL(g)	113.63	0.21					1986CHA
		SEL(l,s)			219.08	0.4	145.9	2.0	1985WIL
			113.93	1.14			146.1	2.0	2019DIK
					221.88				1988OKA
					215.37				1988CAC
							146.11		1963OET
$C_5H_{12}O$	1-pentanol	SEL(g)	130.75	1.31	208.31	0.41			2019DIK
		SEL(l)			208.19	0.30			1986TAN
	2-methyl-1-butanol	SEL	136.2	8.6	213.77	1.84			2019DIK
	isopentanol	SEL	136.2	8.6	209.75	1.66			2019DIK
$C_6H_{14}O$	*n*-hexanol	SEL(g)	153.39	1.53	242.00	1.25			2019DIK
		SEL(l)			240.57				1986TAN
					241.32				1988AND
Sugars									
$C_2H_6O_2$	1,2-ethanediol	SEL(g)	82.7	0.13					1986CHA
		SEL(l)			149.3	0.8			1985WIL
			82.67	0.83	148.75	0.61			2019DIK
$C_3H_8O_3$	glycerin	SEL(g)	124.0	7.6	220.57	0.79			2019DIK
		SEL(l)			206.3	1.0			1985WIL

$C_6H_{12}O_6$	alpha-*D*-glucose	SEL					219.19	0.42	2019DIK
	fructose	SEL					213.15	0.67	2019DIK
$C_{12}H_{22}O_{11}$	sucrose	SEL					424.30	0.82	2019DIK
Cycloalkanols									
$C_5H_{10}O$	cyclopentanol	SEL(g)	113.12	1.13	182.37	0.85			2019DIK
		SEL(l)			184.14				1956PAR
$C_6H_{12}O$	cyclohexanol	SEL	127.65	1.28	209.38	1.63	192.31	0.30	2019DIK
					214.06				1990MAY
			132.70						1988KAB
					209.99				1988CAC
Alkoxyalkanols									
$C_3H_8O_2$	2-methoxyethanol	SEL	106.8	6.4	175.28	1.41			2019DIK
C_7H_8O	4-methylphenol	SEL(g)	124.97	0.50					1978KUD
		SEL(s)					150.25	1.00	1967AND
			125.10	1.25			150.25	1.16	2019DIK
							221.03		1975NIC
Ethers									
C_2H_6O	dimethyl ether	SEL(g)	65.57	0.08					1986CHA
		SEL(l)	65.60	0.66	112.66	1.47			2019DIK
			65.54						1940KIS
$C_4H_{10}O$	diethyl ether	SEL(g)	119.46	0.15					1986CHA
		SEL(l)			172.4	0.2			1985WIL
			119.62	1.20	172.37	0.44			2019DIK
					172.50				1971COU
$C_6H_{14}O$	diisopropyl ether	SEL(g)	158.31	1.58	216.42	0.70			2019DIK
		SEL(l)			216.74				1993GRO
Aldehydes									
CH_2O	formaldehyde	SEL(g)	35.39	0.02					1986CHA
		SEL(l)			82.6	3.0			2019DIK
C_2H_4O	acetaldehyde	SEL(g)	55.32	0.08					1985CHA
		SEL(l)			89.05				1988LEB
					100.8	4.2			2012KRO
C_3H_6O	propanal	SEL(g)	80.73	0.10					1986CHA
		SEL(l)			137.2	1.4			1980FUC
C_4H_8O	butanal	SEL(g)	103.36	0.1					1986CHA
		SEL(l)			163.7	1.0			1985WIL
Alkenyl Aldehydes									

C_3H_4O	1-propenal	SEL	71.46	0.72			2019DIK
C_3H_4O	2-propenal	SEL	71.28	0.71	118.7	3.3	2019DIK
Ketones							
C_3H_6O	acetone	SEL(g)	75.02	0.11			1986CHA
		SEL(l)	74.52	0.75	126.81	0.67	2019DIK
					125.45	1.00	1991MAL
					126.6	1.5	1985WIL
					123.80		1985COS
					128.24		1955STA
C_4H_8O	butanone	SEL(g)	101.68	0.14			1986CHA
		SEL(l)			158.40	0.30	1985COS
			103.27	1.03	158.74	0.41	2019DIK
					158.90	0.4	1985WIL
					158.41		1956PAR
Carboxylic Acids							
CH_2O_2	formic acid	SEL(g)	45.68	0.07			1986CHA
		SEL(l)			99.51	0.2	1985WIL
			45.70	0.46	99.77	0.90	2019DIK
					99.04		1941STO
$C_2H_4O_2$	acetic acid	SEL(g)	63.44	0.11			1978CHA
		SEL(l)			123.10	0.30	1982MAR
			63.46	0.64	123.09	0.38	2019DIK
					123.6	2.0	1985WIL
C_3H_6O	propanoic acid	SEL(g)	87.6	5.4	152.81	0.20	2019DIK
		SEL(l)			152.80		1982MAR
					152.7	2.0	1985WIL
C_4H_8O	*n*-butanoic acid	SEL	110.8	6.9	177.67	0.19	2019DIK
					178.6	1.4	1985WIL
					177.70		1982MAR
					178.00		1971KON
$C_5H_{10}O_2$	n-pentanoic acid	SEL(g)	134.1	8.4	207.8	2.1	2019DIK
		SEL(l)			210.33		1965MCD
					197.00		1971KON
Esters							
$C_2H_4O_2$	methyl formate	SEL(g)	64.38	0.09			1986CHA
		SEL(l)			119.70		1979FUC
			66.61	0.67	119.4	3.5	2019DIK

$C_3H_6O_2$	ethyl formate	SEL(g)	88.64	0.89	143.7	2.5	2019DIK
		SEL(l)			144.30		1979FUC
	methyl acetate	SEL(g)	86.03	0.12			1986CHA
		SEL(l)			141.34		1988PIN
			86.04	0.86	143.09	0.42	2019DIK
					140.60		1985COS
$C_4H_8O_2$	ethyl acetate	SEL(g)	113.66	1.14	168.84	0.62	2019DIK
		SEL(l)			168.94		1988PIN
					170.6	0.5	1985WIL
					169.60		1985COS
					167.40		1979FUC
	methyl propanoate	SEL(g)	116.58	1.17	173.96	0.68	2019DIK
		SEL(l)			174.20		1979FUC
					171.21		1988PIN
	n-propyl formate	SEL(g)	117.6	7.1	171.91	1.88	2019DIK
		SEL(l)			172.10		1988PIN
$C_5H_{10}O_2$	methyl butanoate	SEL(g)	130.7	8.3	197.96	0.25	2019DIK
		SEL(l)			200.80		1979FUC
Alkenyl Esters							
$C_4H_6O_2$	ethenyl acetate	SEL	99.00	0.99	163.7	4.5	2019DIK
$C_5H_8O_2$	ethyl propenoate	SEL	121.2	7.7	184.0	5.2	2019DIK
	methyl 2-methylpropenoate	SEL	122.1	7.7	187.3	5.9	2019DIK
Oxacycloalkanes							
C_2H_4O	oxacyclopropane	SEL(g)	47.0	1.00			1992DOR
		SEL(l)	47.87	0.48	89.56	0.68	2019DIK
C_3H_6O	methyloxacyclopropane	SEL(g)	72.55	0.12			1986CHA
		SEL(l)			120.41	0.35	1985WIL
	oxacyclobutane	SEL(g)	61.50	2.00			1992DOR
		SEL(l)	62.03	1.41	114.5	3.2	2019DIK
C_4H_8O	oxacyclopentane	SEL(g)	76.25	0.16			1986CH
		SEL(l)			124.1	0.2	1985WIL
			76.57	0.77	124.15	0.64	2019DIK
					124.10		1985COS
Oxacycloalkenes							
C_2H_2O	oxacyclopropene	SEL	54.2	3.0			1992DOR
C_4H_4O	oxacyclopentadiene	SEL(g)	65.40	0.29			1986CHA
		SEL(l)			114.56		1952GUT

			65.40	1.50					1992DOR
			65.43	0.65	114.61	0.35			2019DIK
C_4H_6O	1-oxa-3-cyclopentene	SEL(g)	75.60	0.12					1986CHA
		SEL(l)	75.78	0.76	126.3	4.5			2019DIK
			73.21	0.11					1992DOR
Multioxacyclolalkanes									
CH_2O_2	1,2-dioxacyclopropane	SEL(g)	43.9	3.0					1992DOR
$C_2H_4O_2$	1,2-dioxacyclobutane	SEL(g)	77.0	4.0					1992DOR
$C_2H_4O_3$	1,2,3-trioxacyclopentane	SEL(g)	78.0	4.5					1992DOR
$C_3H_6O_2$	1,3-dioxacyclopentane	SEL(g)	71.0	4.0					1992DOR
		SEL(l)	73.9	4.9	121.71	1.19			2019DIK
$C_3H_6O_3$	1,3,5-trioxacyclohexane	SEL	82.36	0.82			113.08	1.37	2019DIK
$C_4H_8O_2$	1,3-dioxane	SEL	89.54	0.90	140.3	2.4			2019DIK
	1,4-dioxane	SEL	92.25	0.92	150.56	0.66			2019DIK
					149.65				1993GRO
					153.6	2.5			1985WIL
Cycloketones									
$C_{10}H_{16}O$	*D*-camphor	SEL	191	13			246.29	0.24	2019DIK
$C_4H_2O_3$	2,5-furandione	SEL	84.6	5.3			119.24	0.17	2019DIK
Aromatic Alcohols									
C_6H_6O	phenol	SEL(g)	103.22						1978KUD
		SEL(s)					127.21		1975NIC
			103.22	1.03			127.45	0.47	2019DIK
C_7H_8O	2-methylphenol	SEL(g)	127.30						1978KUD
		SEL(s)					154.56	1.00	1967AND
			127.30	1.27			154.56	1.25	2019DIK
	3-methylphenol	SEL(g)	124.68						1978KUD
		SEL(l)			224.93	1.30			1967AND
			124.77	1.25	223.3	2.0			2019DIK
	benzyl alcohol	SEL(g)	126.8	8.1	215.9	2.4			2019DIK
		SEL(l)			215.94	1.00			1975NIC
Aromatic Aldehydes									
C_7H_6O	benzaldehyde	SEL(g)	111.70	1.00					1975AMB
		SEL(l)			172.00				1975AMB2
			111.68	1.12	171.99	0.37			2019DIK
Aromatic Carboxylic Acids									
$C_7H_6O_2$	benzoic acid	SEL(g)	124.0	7.9			146.74	1.42	2019DIK

		SEL(s)					147.78	1.00	1993KAJ
			103.47						1969STU
Hydrogen Cyanides									
CHN	hydrogen cyanide	SEL	35.86	0.36	72.95	1.43			2019DIK
Alkyl Amines									
CH_5N	methylamine	SEL	50.08	0.50	104.8	2.7			2019DIK
C_2H_7N	ethylamine	SEL	71.65	0.72					2019DIK
C_3H_9N	1-propylamine	SEL(g)	91.25	0.91	164.35	0.92			2019DIK
		SEL(l)			162.51	1.00			1972FIN
					160.00				1971KON
	isopropylamine	SEL(g)	97.62	0.98	163.84	0.63			2019DIK
		SEL(l)			163.85				1972FIN
					164.00				1971KON
$C_4H_{11}N$	isobutylamine	SEL(g)	117.1	7.5					2019DIK
		SEL(l)			194.00				1971KON
	n-butylamine	SEL(g)	118.52	1.19	188.1	4.5			2019DIK
		SEL(l)			188.00				1971KON
	tert-butylamine	SEL(g)	121.00	1.21	192.06	0.63			2019DIK
		SEL(l)			190.00				1971KON
C_2H_7N	dimethylamine	SEL	70.45	0.70	140.5	2.6			2019DIK
C_3H_9N	methylethylamine	SEL	87.6	5.7					2019DIK
$C_4H_{11}N$	diethylamine	SEL(g)	115.77	1.16	178.09	0.85			2019DIK
		SEL(l)			178.10				1985COS
C_3H_9N	trimethylamine	SEL	91.80	0.92	138.15	0.99			2019DIK
$C_6H_{15}N$	*n*-hexylamine	SEL(g)	164	10	250.5	2.4			2019DIK
		SEL(l)			252.00				1971KON
	triethylamine	SEL(g)	160.98	1.61	221.3	2.3			2019DIK
		SEL(l)			216.43				1993GRO
$C_6H_{13}N$	cyclohexylamine	SEL	132.0	8.7	201.2	8.9			2019DIK
$C_6H_{12}N_4$	methenamine	SEL(s)					152.31	0.55	2019DIK
Alkanenitriles									
C_2H_3N	ethanenitrile	SEL	52.25	0.52	91.22	0.37			2019DIK
C_3H_5N	propanenitrile	SEL	73.77	0.74	120.26	0.89			2019DIK
C_4H_7N	butanenitrile	SEL	94.51	0.95	133.50	1.88			2019DIK
C_3H_3N	propenenitrile	SEL	63.93	0.64	108.48	0.49			2019DIK
Cyanogens									
C_2N_2	cyanogen	SEL	56.92	0.57	113.9	4.7			2019DIK

Hydrazines									
$C_2H_8N_2$	1,1-dimethylhydrazine	SEL	89.7	5.7	164.06	0.67			2019DIK
Aromatic Amines									
$C_3H_6N_6$	melamine	SEL	137.8	8.5			155.16	0.75	2019DIK
C_6H_7N	aniline	SEL(g)	108.14	1.08	192.42	0.82			2019DIK
		SEL(l)			191.01	1.20			1975NIC
$C_8H_{11}N$	*N*,*N*-dimethylaniline	SEL	151.2	9.8	211.9	5.6			2019DIK
Ureas									
CH_4N_2O	urea	SEL	77.55	0.78			92.79	0.32	2019DIK
Oxyamines									
$C_6H_{15}NO_3$	triethanolamine	SEL	213	13	361	21			2019DIK
Nitrates and Nitrites									
CH_3NO_3	methyl nitrate	SEL(g)	76.49	0.77	152.1	7.1			2019DIK
		SEL(l)			157.19				1953GRA
$C_3H_5N_3O_9$	nitroglycerin	SEL	234.5	2.6					2019DIK
CN_4O_8	tetranitromethane	SEL	171.6	5.4	207	11			2019DIK
CHN_3O_6	trinitromethane	SEL	131.5	3.8	182	11			2019DIK
CH_3NO_2	nitromethane	SEL(g)	57.27	0.57	106.25	0.78			2019DIK
		SEL(l)			105.98				1947JON
Isocyano Aromatics									
$C_9H_6N_2O_2$	2,4-diisocyanatotoluene	SEL			287.80				2019DIK
Nitro Aromatics									
$C_6H_3N_3O_6$	trinitrobenzene	SEL(g)	197.48	1.97			222.67	5.81	2019DIK
		SEL(s)					214.60		1980RAD
$C_6H_5NO_2$	nitrobenzene	SEL(g)	119.57	1.20	182.1	2.2			2019DIK
		SEL(l)			181.13				1985LAI
$C_7H_5N_3O_6$	trinitrotoluene	SEL(g)	213.3	5.6			236.80	12.30	2019DIK
		SEL(s)					243.30		1991YIN
Alkanethiols									
CH_4S	methanethiol	SEL	50.31	0.50	90.47	0.63			2019DIK
C_2H_6S	ethanethiol	SEL(g)	73.02	0.73	117.82	0.24			2019DIK
		SEL(l)			117.99				1952MCC
Alkyl Sulfides									
CS_2	carbon disulfide	SEL(g)	45.51	0.46	78.14	0.62			2019DIK
		SEL(l)			78.99	0.80			1955STA
C_2H_6S	dimethyl sulfide	SEL	74.08	0.74	118.28	0.84			2019DIK
C_2H_6OS	dimethyl sulfoxide	SEL(g)	89.43	0.89	150.97	1.05			2019DIK

		SEL(l)			149.39		1993GRO
Fluoroalkanes							
CH_3F	fluoromethane	SEL(g)	37.49				1998CHA
		SEL(l)			106.26	1.09	1998HO
			37.49	0.38	105.89	0.91	2019DIK
			37.52	0.36			1965BAR
CH_2F_2	difluoromethane	SEL(g)	42.83				1998CHA
		SEL(l)			97.26	0.80	1996LUD
			42.90	0.43	97.33	0.42	2019DIK
			43.18	0.43			1965BAR
CHF_3	trifluoromethane	SEL	51.04	0.30			1962VAL
			51.01	0.51			2019DIK
			50.99				1998CHA
			51.38	0.51			1965BAR
CF_4	tetrafluoromethane	SEL	61.02				1998CHA
			61.04	0.61			2019DIK
			61.07	0.03			1989EWI
			61.55	0.60			1965BAR
C_2H_5F	fluoroethane	SEL	59.62	0.60	108.9	5	2018LEM
			59.65	0.60	112.2	5.3	2019DIK
$C_2H_4F_2$	1,1-difluoroethane	SEL	67.48	0.67	118.9	1.2	2018LEM
			68.49	0.69	118.38	0.21	2019DIK
$C_2H_4F_2$	1,2-difluoroethane	SEL	67.77	0.68	217.0	7.2	2019DIK
$C_2H_3F_3$	1,1,1-trifluoroethane	SEL	78.08	0.16	140.24	0.70	2018LEM
	1,1,2-trifluoroethane	SEL	77.42	0.77	137.5	4.6	2019DIK
$C_2H_2F_4$	1,1,1,2-tetrafluoroethane	SEL	85.03	0.21	145.36	0.73	2018LEM
			86.69	0.87	143.55	0.74	2019DIK
	1,1,2,2-tetrafluoroethane	SEL	90.35	0.90	147.7	5.8	2019DIK
C_2HF_5	pentafluoroethane	SEL	94.44	0.94	166.0	6.7	2019DIK
C_2F_6	hexafluoroethane	SEL	106.61	1.07			2019DIK
Fluoroalkenes							
C_2H_3F	fluoroethene	SEL	50.43	0.50	99.1	6.7	2019DIK
$C_2H_2F_2$	1,1-difluoroethene	SEL	59.08	0.59			2019DIK
	1,2-difluoroethene, (E)-	SEL	60.26	0.60	129.9	8.0	2019DIK
	1,2-difluoroethene, (Z)-	SEL	58.35	0.58	103.5	5.5	2019DIK
C_2HF_3	trifluoroethene	SEL	69.20	0.69	145	11	2019DIK
C_2F_4	tetrafluoroethene	SEL	80.42	0.80			2019DIK

Chloroalkanes							
CH_3Cl	chloromethane	SEL(g)	40.74	0.41	81.44	0.72	2019DIK
		SEL(l)			81.70	0.50	1940AWB
			42.07	1.69			1964SEN
					81.20		1924SHO
CH_2Cl_2	dichloromethane	SEL(g)	50.85				1998CHA
		SEL(l)			98.6	2.4	2015CHO
			50.90	0.51	100.13	0.91	2019DIK
					97.97	1.96	2008TJA
					102.27	0.71	1978MOS
			51.60	0.48			1965BAR
			52.6	2.1			1964SEN
					99.50	0.36	1943MCG
					100.0	3.2	1940RIE
					100.59	1.00	1937PERE
$CHCl_3$	trichloromethane	SEL(g)	65.33				1998CHA
		SEL(l)			113.20		1993SHE
			65.36	0.65	114.43	0.47	2019DIK
					114.25		1993GRO
			65.87	0.61			1965BAR
					114.18		1955STA
CCl_4	tetrachloromethane	SEL(g)	82.65				1998CHA
		SEL(l)			131.34		1982TAN
			83.46	0.84	131.74	0.41	2019DIK
					131.30		1993SHE
					132.59		1955STA
					131.69	0.46	1944HIC
					132.7	8.0	1937STU
C_2H_5Cl	chloroethane	SEL	62.65	0.63	105.31	0.81	2019DIK
$C_2H_4Cl_2$	1,1-dichloroethane	SEL	76.33	0.76	126.44	0.63	2019DIK
	1,2-dichloroethane	SEL	77.32	0.77	129.19	0.52	2019DIK
$C_2H_3Cl_3$	1,1,1-trichloroethane	SEL	92.33	0.92	144.37	0.81	2019DIK
	1,1,2-trichloroethane	SEL	84.94	0.85	141.4	5.1	2019DIK
$C_2H_2Cl_4$	1,1,1,2-tetrachloroethane	SEL	102.88	1.03	157.9	6.1	2019DIK
	1,1,2,2-tetrachloroethane	SEL(g)	98.97	0.99	165.62	0.83	2019DIK
		SEL(l)			168.00		1989WIL
C_2HCl_5	pentachloroethane	SEL	118.07	1.18	174.3	7.2	2019DIK

C_2Cl_6	hexachloroethane	SEL	136.78	1.37			198.24	1.64	2019DIK
Chloroalkenes									
C_2H_3Cl	chloroethene	SEL	53.60	0.54	96.2	3.3			2019DIK
$C_2H_2Cl_2$	1,1-dichloroethene	SEL	66.93	0.67	110.80	0.67			2019DIK
	1,2-dichloroethene, (E)-	SEL	66.55	0.67	113.83	1.18			2019DIK
	1,2-dichloroethene, (Z)-	SEL	65.00	0.65	112.85	1.12			2019DIK
C_2HCl_3	trichloroethene	SEL	79.75	1.00	128.70	1.13			2019DIK
C_2Cl_4	tetrachloroethene	SEL(g)	95.51						1993GRO
		SEL(l)			147.16				1989WIL
			94.88	0.95	151.92	1.94			2019DIK
Chloroalkynes									
C_2HCl	chloroethyne	SEL	51.6	2.8	135.5	4.4			2019DIK
C_2Cl_2	dichloroethyne	SEL	61.1	3.2	185.1	8.0			2019DIK
Chloro Aromatic									
C_6H_5Cl	chlorobenzene	SEL(g)	97.99	0.98	150.87	1.14			2019DIK
		SEL(l)			152.10				1993SHE
Bromoalkanes									
CH_3Br	bromomethane	SEL	42.45	0.43	81.59	1.21			2019DIK
CH_2Br_2	dibromomethane	SEL(g)	54.59	0.55	104.48	0.88			2019DIK
		SEL(l)			104.1	3.1			1993SHE
					105.15	0.41			1957HAR
$CHBr_3$	tribromomethane	SEL	70.99	0.71	121.5	6.3			2019DIK
					135.10				1932TRE
CBr_4	tetrabromomethane	SEL(g)	90.71						1998CHA
		SEL(s)					145.90		1984BIC
			91.13	0.91			127.78	0.51	2019DIK
C_2H_5Br	bromoethane	SEL(g)	64.27	0.64	107.38	0.81			2019DIK
		SEL(l)			105.80				1993SHE
C_2H_3Br	bromoethene	SEL(g)	55.49	0.56					2019DIK
		SEL(l)			114.3	3.7			2012KRO
Iodoalkanes									
CH_3I	iodomethane	SEL(g)	44.08	0.44	82.58	0.61			2019DIK
		SEL(l)			82.75				1993CAR
					82.00				1993SHE
CH_2I_2	diiodomethane	SEL(g)	57.75	0.58	112.6	5.8			2019DIK
		SEL(l)			112.80				1993SHE
					133.81				1993CAR

CHI_3	triiodomethane	SEL(g)	75.06	0.75			2019DIK
		SEL(l)			157.50		1993CAR
CI_4	tetraiodomethane	SEL(g)	95.78	0.96			2019DIK
		SEL(l)			259.80		1993CAR
Chlorofluoroalkanes							
CH_2ClF	chlorofluoromethane	SEL(g)	47.29	0.46			1965BAR
		SEL(l)	47.08	0.47	73.2	2.4	2019DIK
$CHCl_2F$	dichlorofluoromethane	SEL(g)	61.33	0.64			1965BAR
		SEL(l)	60.95	0.61	107.5	3.8	2019DIK
$CHClF_2$	chlorodifluoromethane	SEL(g)	56.00	0.22			1995ESP
		SEL(l)			107.2	3.2	1940BEN
			55.87	0.56	108.5	2.5	2019DIK
			56.35	0.06			1970ERN
			56.17	0.60			1965BAR
CCl_2F_2	dichlorodifluoromethane	SEL(g)	73.92	0.21			1991BUF
		SEL(l)	72.30	0.72	119.9	4.8	2019DIK
			73.66	0.47			1969SHU
			72.94	0.73			1965BAR
CCl_3F	trichlorofluoromethane	SEL(g)	78.09	0.78	121.67	0.83	2019DIK
		SEL(l)			121.55	0.46	1941OSB
			74.64	0.76			1965BAR
					123.6	3.6	1940BEN
$CClF_3$	chlorotrifluoromethane	SEL	66.87	0.67			2019DIK
C_2ClF_3	chlorotrifluoroethene	SEL	83.94	0.84	137.0	2.7	2019DIK
Bromofluoroalkanes							
CH_2BrF	bromofluoromethane	SEL	49.14	0.49	114.3	3.8	2019DIK
$CHBrF_2$	bromodifluoromethane	SEL	58.78	0.59	106.5	3.8	2019DIK
CBr_2F_2	dibromodifluoromethane	SEL	77.02	0.77	118.6	3.6	2019DIK
CBr_3F	tribromofluoromethane	SEL	84.37	0.84	169.7	6.4	2019DIK
$CBrF_3$	bromotrifluoromethane	SEL	69.26	0.69	125.24	0.27	2019DIK
Bromochloroalkanes							
CH_2BrCl	bromochloromethane	SEL(g)	52.76	0.53	103.90	1.22	2019DIK
		SEL(l)			104.1	2.6	2015CHO
$CHBr_2Cl$	dibromochloromethane	SEL	69.15	0.69	129.3	5.2	2019DIK
$CHBrCl_2$	bromodichloromethane	SEL	67.25	0.67	115.9	3.6	2019DIK
CBr_2Cl_2	dibromodichloromethane	SEL	87.15	0.87	140.43	1.08	2019DIK
$CBrCl_3$	bromotrichloromethane	SEL	85.38	0.85	135.29	0.56	2019DIK

Bromochlorofluoroalkanes							
$CHBrClF$	bromochlorofluoromethane	SEL	62.85	0.63	103.9	3.6	2019DIK
CBr_2ClF	dibromochlorofluoromethane	SEL	82.33	0.82	130.0	4.8	2019DIK
$CBrCl_2F$	bromodichlorofluoromethane	SEL	80.06	0.80	126.4	4.4	2019DIK
$CBrClF_2$	bromochlorodifluoromethane	SEL	74.66	0.75	118.8	3.9	2019DIK
Carbonyl Halides							
CCl_2O	phosgene	SEL(g)	57.69	0.58			1998CHA
		SEL(l)	57.69	0.58	104.08	0.97	2019DIK
Chloroaromatic Alcohols							
C_6HCl_5O	pentachlorophenol	SEL(g)	189.80	1.90			2019DIK
		SEL(l)			201.96		1958HIL
Siloxanes							
$C_6H_{18}OSi_2$	hexamethyldisiloxane	SEL			311.38	0.82	2019DIK
$C_8H_{24}O_4Si_4$	octamethylcyclotetrasiloxane	SEL			495.9	9.5	2019DIK

5.3. **Recommended Heat Capacities**

This Table 5-2 provides the selected recommended values for heat capacities in the gas, liquid, and solid phases. All the heat capacities that were compiled are provided previously in Table 5-1.

Table 5-8. Recommended heat capacities in gas, liquid, and solid phases

Table 5-3(1). Small Molecules

Formula	Compound	SEL	C_p(g)	$U(C_p g)$	C_p(l)	$U(C_p l)$	C_p(s)	$U(C_p s)$	Reference
			J mol^{-1} K^{-1}						
Hydrogen/Oxygen									
H_2	hydrogen	SEL	28.83	0.29					2019DIK
O_2	oxygen	SEL	29.39						1998CHA
H_2O	water	SEL(g,l)	33.59	0.07	75.33	0.01			2018LEM
		SEL(s)					37.77	0.38	2006FEI
H_2O_2	hydrogen peroxide	SEL	42.36	0.42			59.10	0.20	2019DIK
Nitrogen/Hydrogen/Oxygen									
N_2	nitrogen	SEL	29.09	0.12					1995ESP
H_3N	ammonia	SEL(g)	35.64	0.20					1998CHA
		SEL(l)			81.4	0.8			2018LEM
H_4N_2	hydrazine	SEL	49.14	0.49	98.67	0.39			2019DIK
HN_3	hydrogen azide	SEL	44.22	0.35					1989GUR
N_2O	nitrous oxide	SEL	38.54	0.39					2019DIK
ClH_4NO_4	ammonium perchlorate	SEL					128.07	0.33	1969WES
Sulfur/Hydrogen									
H_2S	hydrogen sulfide	SEL(g)	34.20	0.20					1998CHA
		SEL(l)			75.8	3.2			2019DIK
Boron/Hydrogen									
B_2H_6	diborane	SEL	58.07						1998CHA

Table 5-3(2). Hydrocarbons

Formula	Compound	SEL	C_p(g)	$U(C_p$g) J mol^{-1} K^{-1}	C_p(l)	$U(C_p$l)	C_p(s)	$U(C_p$s)	Reference
Carbon									
C	carbon (gas)	SEL	20.79	0.00					definition
	graphite	SEL					8.43		1980TAY
Alkanes									
CH_4	methane	SEL	35.69	0.20					1989GUR
C_2H_6	ethane	SEL(g)	52.49	0.20					1989GUR
		SEL(l)			160.6	1.9			2019DIK
C_3H_8	propane	SEL(g)	73.60	0.20					1973CHA
		SEL(l)			117.41	0.86			2019DIK
C_4H_{10}	isobutane	SEL(g)	96.65	0.20					1975CHE
		SEL(l)			140.69	0.29			2019DIK
	n-butane	SEL(g)	98.49	0.20					1975CHE
		SEL(l)			140.50	0.87			2019DIK
C_5H_{12}	isopentane	SEL(g)	118.90	0.40					1974SCO
		SEL(l)			164.84	0.73			2019DIK
	neopentane	SEL(g)	120.83	0.25					1974SCO
		SEL(l)			169.2	6.3			2019DIK
	n-pentane	SEL(g)	120.00	0.10					1974SCO
		SEL(l)			167.19				1967MES
C_6H_{14}	2,3-dimethylbutane	SEL(g)	139.40	0.70					1974SCO
		SEL(l)			189.02				1989OHN
	3-methylpentane	SEL(g)	140.10	0.40					1974SCO
		SEL(l)			191.16				1989OHN
	isohexane	SEL(g)	142.2	0.2					1974SCO
		SEL(l)			193.88				1989OHN
	neohexane	SEL(g)	141.5	0.30					1974SCO
		SEL(l)			189.67				1989OHN
	n-hexane	SEL(g)	142.6	0.20					1974SCO
		SEL(l)			195.52				1989OHN
C_7H_{16}	isoheptane	SEL(g)	164.50	0.20					1974SCO
		SEL(l)			222.92	0.45			1961HUF
	neoheptane	SEL(g)	166.70	0.40					1974SCO
		SEL(l)			221.12	0.42			1961HUF

	n-heptane	SEL(g)	165.20	0.30			1974SCO
		SEL(l)			224.73	0.12	1988SHI
C_8H_{18}	2,2,4-trimethylpentane	SEL(g)	188.40	0.40			1974SCO
		SEL(l)			238.87	1.1	1976FOR
	2-methylheptane	SEL(g)	187.2	0.2			1974SCO
		SEL(l)			252.0	0.4	1971MES
	n-octane	SEL(g)	187.8	0.4			1987SCO
		SEL(l)			254.18	1.0	1985LAI2
C_9H_{20}	*n*-nonane	SEL(g)	210.4	0.5			1974SCO
		SEL(l)			284.39	0.5	1954FIN
$C_{10}H_{22}$	*n*-decane	SEL	233.1	0.6			1974SCO
		SEL(l)			314.2	1.4	1984ROU
$C_{16}H_{34}$	*n*-hexadecane	SEL(g)	369.2	3.7			2019DIK
		SEL(l)			499.7	1.0	1981GRO
Alkenes							
C_2H_4	ethene	SEL	43.29	0.30			1941BUR
C_3H_6	propene	SEL(g)	63.79	0.13			1974BIE
		SEL(l)			102.00		1983CHA
C_4H_8	1-butene	SEL(g)	85.65	0.86			2019DIK
		SEL(l)			128.96	0.40	1991TAK
	2-butene, (*E*)-	SEL(g)	87.78	0.40			1940KIS2
		SEL(l)			130.0	2.2	2019DIK
	2-butene, (*Z*)-	SEL(g)	81.13	0.16			1944SCO
		SEL(l)			127.00	0.50	1983CHA
	isobutene	SEL	88.13	0.88	133.6	4.2	2019DIK
C_5H_{10}	1-pentene	SEL(g)	108.16	1.08			2019DIK
		SEL(l)			154.87	0.30	1990MES
	2-methyl-1-butene	SEL(g)	109.98	1.10			2019DIK
		SEL(l)			157.3	0.8	1983CHA
	2-methyl-2-butene	SEL(g)	104.99	1.05			2019DIK
		SEL(l)			152.8	0.7	1983CHA
	2-pentene, (E)-	SEL	108.89	1.09	156.97	0.63	2019DIK
	2-pentene, (Z)-	SEL	98.79	0.99	151.58	0.65	2019DIK
	3-methyl-1-butene	SEL	114.48	1.14	156.16	0.68	2019DIK
C_6H_{12}	1-hexene	SEL	130.82	1.31	183.08	0.55	2019DIK
C_7H_{14}	1-heptene	SEL	153.46	1.53	211.86	0.49	2019DIK
C_8H_{16}	1-octene	SEL	176.17	1.76	241.30	0.43	2019DIK

Alkadienes							
C_3H_4	allene	SEL(g)	59.07	0.24			1940KIS
		SEL(l)	59.06	0.59	102.0	3.7	2019DIK
C_4H_6	1,2-butadiene	SEL	79.50	0.80	123.83	0.86	2019DIK
	1,3-butadiene	SEL	79.64	0.80	123.66	0.48	2019DIK
C_5H_8	1,2-pentadiene	SEL	100.98	1.01	150.84	1.25	2019DIK
	1,3-pentadiene	SEL	98.9	6.3	148.6	4.9	2019DIK
	1,4-pentadiene	SEL	98.34	0.98	146.99	1.23	2019DIK
	2-methyl-1,3-butadiene	SEL	102.76	1.03	150.85	1.37	2019DIK
Alkynes							
C_2H_2	acetylene	SEL	44.04	0.30			1989GUR
C_3H_4	propyne	SEL(g)	60.79				1940KIS
		SEL(l)			109.4	4.1	2019DIK
C_4H_6	1-butyne	SEL	81.37	0.81	135.24	1.05	2019DIK
C_5H_8	1-pentyne	SEL	102.67	1.03	143.3	4.0	2019DIK
	2-pentyne	SEL	99.72	1.00	129.6	3.5	2019DIK
C_6H_{10}	1-hexyne	SEL	128.94	1.29	184.8	5.1	2019DIK
	2-hexyne	SEL	119.65		170.8	4.8	2019DIK
	3-hexyne	SEL	119.5	1.2	179.3	5.0	2019DIK
C_4H_4	butenyne	SEL	73.20	0.73	118.4	3.9	2019DIK
C_5H_6	3-penten-1-yne	SEL	96.3	5.9	139.5	4.7	2019DIK
C_4H_2	butadiyne	SEL(g)	73.7	1.0			1991DOR
		SEL(l)			117.0	3.6	2019DIK
Cycloalkanes							
C_3H_6	cyclopropane	SEL(g)	55.6	1.0			1986DOR2
		SEL(l)			96.37	1.42	2019DIK
C_4H_8	cyclobutane	SEL(g)	70.60	1.50			1986DOR2
		SEL(l)	70.66	0.71	109.89	0.75	2019DIK
C_5H_{10}	cyclopentane	SEL(g)	82.80	2.00			1986DOR2
		SEL(l)			126.74		1985TAN
	methylcyclobutane	SEL	98.79	0.99	145.7	4.9	2019DIK
C_6H_{12}	cyclohexane	SEL(g)	105.30	2.00			1986DOR2
		SEL(l)			156.90		1989LAI
	methylcyclopentane	SEL	109.51	1.10	158.81	0.65	2019DIK
C_7H_{14}	methylcyclohexane	SEL(g)	136.13	1.36			2019DIK
		SEL(l)			184.96	0.5	1985TAN
$C_{10}H_{20}$	1,3-diethylcyclohexane	SEL	204	13	270	11	2019DIK

Cyclopropanes							
C_3H_4	cyclopropene	SEL(g)	52.90	1.00			1986DOR2
		SEL(l)			95.8	3.7	2019DIK
C_4H_6	cyclobutene	SEL(g)	64.40	2.00			1986DOR2
		SEL(l)			101.0	3.4	2019DIK
C_5H_8	cyclopentene	SEL(g)	81.3	2.00			1986DOR2
		SEL(l)			122.38		1948HUF
	methylenecyclobutane	SEL	87.36	0.87	131.56	0.46	2019DIK
C_6H_{10}	cyclohexene	SEL(g)	101.5	3.0			1986DOR2
		SEL(l)			148.80		1991STE
Cycloalkadienes							
C_4H_4	cyclobutadiene	SEL(g)	61.0	2.5			1986DOR2
		SEL(l)				3.7	2019DIK
C_5H_6	cyclopentadiene	SEL(g)	75.4	2.00			1986DOR2
		SEL(l)			119.9	3.4	2019DIK
C_6H_8	1,3-cyclohexadiene	SEL(g)	94.2	2.5			1986DOR2
		SEL(l)			143.7	2.4	2019DIK
	1,4-cyclohexadiene	SEL(g)	94.1	3.0			1986DOR2
		SEL(l)			145.6	2.6	2019DIK
Bicycloalkanes							
$C_{10}H_{18}$	cis-decalin	SEL(g)	168.60	1.00			1988DOR
		SEL(l)			229.17		1989OHN
	trans-decalin	SEL(g)	168.57	1.69			2019DIK
		SEL(l)			232.08		1989OHN
$C_{12}H_{22}$	cyclohexylcyclohexane	SEL	218	15	286.96	0.19	2019DIK

Table 5-3(3). Aromatic Hydrocarbons

Formula	Compound	SEL	C_p(g)	$U(C_p g)$ J mol^{-1} K^{-1}	C_p(l)	$U(C_p l)$	C_p(s)	$U(C_p s)$	Reference
Alkyl Benzenes									
C_6H_6	benzene	SEL(g)	82.2	0.20					2014RUZ
		SEL(l)			135.69	0.30			1993GRO
C_7H_8	toluene	SEL(g)	103.7	0.40					1985DRA
		SEL(l)			157.09	0.30			1993GRO
C_8H_{10}	1,2-dimethylbenzene	SEL(g)	132.5	0.40					1985DRA
		SEL(l)			187.65	0.3			1979FOR
	1,3-dimethylbenzene	SEL(g)	125.80	0.40					1985DRA
		SEL(l)			184.63				1993GRO
	1,4-dimethylbenzene	SEL(g)	125.6	0.40					1985DRA
		SEL(l)			181.94	0.3			1979FOR
	ethylbenzene	SEL(g)	127.5	0.2					1978MIL
		SEL(l)			185.87	0.20			1997CHI
C_9H_{12}	isopropylbenzene	SEL	159.75	1.60	215.21	0.52			2019DIK
$C_{10}H_{14}$	2-isopropyltoluene	SEL	180	12	251.4	8.3			2019DIK
	3-isopropyltoluene	SEL	180	12	250.4	8.0			2019DIK
	4-isopropyltoluene	SEL	180	12	238.5	2.8			2019DIK
Alkenyl Benzenes									
C_8H_8	ethenylbenzene	SEL(g)	120.27	1.20					2019DIK
		SEL(l)			182.60				1961WAR
Benzocycloalkanes									
C_9H_{10}	benzocyclopentane	SEL(g)	130.7	1.00					1986DOR
		SEL(l)			189.66	0.21			2019DIK
$C_{10}H_{12}$	benzocyclohexane	SEL(g)	150.9	2.00					1988DOR
		SEL(l)			217.44				1957MCC
Naphthalenes									
$C_{10}H_8$	naphthalene	SEL(g)	131.94	1.32			165.69	0.46	2019DIK
		SEL(l)			196.06				1993CHI
		SEL(s)					165.69		1957MCC
$C_{11}H_{10}$	1-methylnaphthalene	SEL(g)	159.59	1.60					2019DIK
		SEL(l)			224.39				1957MCC
	2-methylnaphthalene	SEL(g)	159.83	1.60					2019DIK
		SEL(l)			195.98	0.6			1957MCC

Polycyclic Aromatic								
$C_{12}H_8$	acenaphthylene	SEL(g)	154.80	1.00				1986DOR
		SEL(s)	154.79	1.55		183	15	2019DIK
	biphenylene	SEL	159.35	1.59				2019DIK
$C_{12}H_{10}$	acenaphthene	SEL(g)	162.20	1.00				1986DOR
		SEL(s)				190.37	0.50	1977FIN
$C_{13}H_{10}$	fluorene	SEL(g)	173.10	1.00				1989DOR
		SEL(s)				203.13		1977FIN
$C_{14}H_8$	pyracyclene	SEL	172.50	1.50				1986DOR
$C_{14}H_{10}$	anthracene	SEL(g)	184.70	1.00				1988DOR
		SEL(s)				211.70	1.00	1980RAD
	phenanthrene	SEL(g)	185.70	1.86		220.63	0.54	2019DIK
		SEL(s)				220.62		1977FIN
$C_{14}H_{12}$	pyracene	SEL	187.20	1.50				1986DOR
$C_{16}H_{10}$	aceanthrylene	SEL(g)	203.00	1.50				1986DOR
		SEL(l)			334 18			2019DIK
	fluoranthene	SEL(g)	203.60	2.00				1989DOR
		SEL(s)				230.25		1971WON
	pyrene	SEL(g)	204.20					1988DOR
		SEL(s)				229.36		1980SMI
$C_{18}H_{12}$	naphthacene	SEL(g)	233.40	1.50				1988DOR
		SEL(s)				236.60		1980WON
	triphenylene	SEL(g)	222.1	2.2		259.20	0.33	2019DIK
		SEL(s)				229.70		1971WON
$C_{20}H_{12}$	perylene	SEL(g)	255.4	2.4				1988DOR
		SEL(s)				274.93	0.46	1980WON
$C_{24}H_{12}$	coronene	SEL(g)	286.6	5.0				1988DOR
		SEL(s)				313.80	1.00	1980WON

Table 5-3(4). Oxidized Hydrocarbons

Formula	Compound	SEL	C_p(g)	$U(C_p g)$ J mol^{-1} K^{-1}	C_p(l)	$U(C_p l)$	C_p(s)	$U(C_p s)$	Reference
Carbon Oxides									
CO	carbon monoxide	SEL	29.14	0.15					1998CHA
CO_2	carbon dioxide	SEL	37.14	0.16	284.63	1.06			2018LEM
Alkanols									
CH_4O	methanol	SEL(g)	44.04	0.03					1986CHA
		SEL(l)			81.08	0.20			1985WIL
C_2H_6O	ethanol	SEL(g)	65.20	0.14					1986CHA
		SEL(l)			112.25	0.30			1985WIL
C_3H_8O	1-propanol	SEL(g)	85.56	0.14					1986CHA
		SEL(l)			143.74	0.4			1985WIL
	isopropanol	SEL(g)	89.32	0.15					1986CHA
		SEL(l)			155.0	0.3			1985WIL
$C_4H_{10}O$	1-butanol	SEL(g)	108.03	0.25					1986CHA
		SEL(l)			177.06	0.35			1985WIL
	2-butanol	SEL(g)	112.74	0.17					1986CHA
		SEL(l)			196.89	0.25			1985WIL
	isobutanol	SEL(g)	113	7					2019DIK
		SEL(l)			181.16	0.4			1985WIL
	tert-butanol	SEL(g)	113.63	0.21					1986CHA
		SEL(l,s)			219.08	0.4	145.9	2.0	1985WIL
$C_5H_{12}O$	1-pentanol	SEL(g)	130.75	1.31					2019DIK
		SEL(l)			208.19	0.30			1986TAN
	2-methyl-1-butanol	SEL	136.2	8.6	213.77	1.84			2019DIK
	isopentanol	SEL	136.2	8.6	209.75	1.66			2019DIK
$C_6H_{14}O$	*n*-hexanol	SEL(g)	153.39	1.53					2019DIK
		SEL(l)			240.57	1.5			1986TAN
Sugars									
$C_2H_6O_2$	1,2-ethanediol	SEL(g)	82.7	0.13					1986CHA
		SEL(l)			149.3	0.8			1985WIL
$C_3H_8O_3$	glycerin	SEL(g)	124.0	7.6					2019DIK
		SEL(l)			206.3	1.0			1985WIL
$C_6H_{12}O_6$	alpha-*D*-glucose	SEL					219.19	0.42	2019DIK
	fructose	SEL					213.15	0.67	2019DIK

$C_{12}H_{22}O_{11}$	sucrose	SEL					424.30	0.82	2019DIK
Cycloalkanols									
$C_5H_{10}O$	cyclopentanol	SEL(g)	113.12	1.13					2019DIK
		SEL(l)			184.14				1956PAR
$C_6H_{12}O$	cyclohexanol	SEL	127.65	1.28	209.38	1.63	192.31	0.30	2019DIK
Alkoxyalkanols									
$C_3H_8O_2$	2-methoxyethanol	SEL	106.8	6.4	175.28	1.41			2019DIK
C_7H_8O	4-methylphenol	SEL(g)	124.97	0.50					1978KUD
		SEL(s)					150.25	1.00	1967AND
Ethers									
C_2H_6O	dimethyl ether	SEL(g)	65.57	0.08					1986CHA
		SEL(l)			112.7	1.5			2019DIK
$C_4H_{10}O$	diethyl ether	SEL(g)	119.46	0.15					1986CHA
		SEL(l)			172.4	0.2			1985WIL
$C_6H_{14}O$	diisopropyl ether	SEL(g)	158.3	1.6					2019DIK
		SEL(l)			216.7	0..7			1993GRO
Aldehydes									
CH_2O	formaldehyde	SEL(g)	35.39	0.02					1986CH
		SEL(l)			82.6	3.0			2019DIK
C_2H_4O	acetaldehyde	SEL(g)	55.32	0.08					1985CHA
		SEL(l)			89.05				1988LEB
C_3H_6O	propanal	SEL(g)	80.73	0.10					1986CHA
		SEL(l)			137.20	1.40			1980FUC
C_4H_8O	butanal	SEL(g)	103.36	0.1					1986CHA
		SEL(l)			163.7	1.0			1985WIL
Alkenyl Aldehydes									
C_3H_4O	1-propenal	SEL	71.46	0.72					2019DIK
C_3H_4O	2-propenal	SEL	71.28	0.71	118.7	3.3			2019DIK
Ketones									
C_3H_6O	acetone	SEL(g)	75.02	0.11					1986CHA
		SEL(l)			126.8	0.7			2019DIK
C_4H_8O	butanone	SEL(g)	101.68	0.14					1986CHA
		SEL(l)			158.40	0.30			1985COS
Carboxylic Acids									
CH_2O_2	formic acid	SEL(g)	45.68	0.07					1986CHA
		SEL(l)			99.51	0.2			1985WIL
$C_2H_4O_2$	acetic acid	SEL(g)	63.44	0.11					1978CHA

		SEL(l)			123.10	0.30	1982MAR
C_3H_6O	propanoic acid	SEL(g)	87.6	5.4			2019DIK
		SEL(l)			152.80	0.2	1982MAR
C_4H_8O	*n*-butanoic acid	SEL	110.8	6.9	177.67	0.19	2019DIK
$C_5H_{10}O_2$	*n*-pentanoic acid	SEL(g)	134.1	8.4			2019DIK
		SEL(l)			210.33	2.0	1965MCD
Esters							
$C_2H_4O_2$	methyl formate	SEL(g)	64.38	0.09			1986CHA
		SEL(l)			119.70		1979FUC
$C_3H_6O_2$	ethyl formate	SEL(g)	88.64	0.89			2019DIK
		SEL(l)			144.30		1979FUC
	methyl acetate	SEL(g)	86.03	0.12			1986CHA
		SEL(l)			141.34		1988PIN
$C_4H_8O_2$	ethyl acetate	SEL(g)	113.66	1.14			2019DIK
		SEL(l)			168.94	0.6	1988PIN
	methyl propanoate	SEL(g)	116.58	1.17			2019DIK
		SEL(l)			174.20	0.7	1979FUC
	n-propyl formate	SEL(g)	117.6	7.1			2019DIK
		SEL(l)			172.10	1.5	1988PIN
$C_5H_{10}O_2$	methyl butanoate	SEL(g)	130.7	8.3			2019DIK
		SEL(l)			200.80	0.6	1979FUC
Alkenyl Esters							
$C_4H_6O_2$	ethenyl acetate	SEL	99.00	0.99	163.7	4.5	2019DIK
$C_5H_8O_2$	ethyl propenoate	SEL	121.2	7.7	184.0	5.2	2019DIK
	methyl 2-methylpropenoate	SEL	122.1	7.7	187.3	5.9	2019DIK
Oxacycloalkanes							
C_2H_4O	oxacyclopropane	SEL(g)	47.0	1.00			1992DOR
		SEL(l)			89.56	0.68	2019DIK
C_3H_6O	methyloxacyclopropane	SEL(g)	72.55	0.12			1985CHA
		SEL(l)			120.41	0.35	1985WIL
	oxacyclobutane	SEL(g)	61.50	2.00			1992DOR
		SEL(l)			114.5	3.2	2019DIK
C_4H_8O	oxacyclopentane	SEL(g)	76.57	0.77			2019DIK
		SEL(l)			124.10	0.6	1985COS
Oxacycloalkenes							
C_2H_2O	oxacyclopropene	SEL	54.2	3.0			1992DOR
C_4H_4O	oxacyclopentadiene	SEL(g)	65.40	0.29			1986CHA

		SEL(l)			114.56				1952GUT
C_4H_6O	1-oxa-3-cyclopentene	SEL(g)	73.21	0.11					1992DOR
		SEL(l)			126.3	4.5			2019DIK
Multioxacyclolalkanes									
CH_2O_2	1,2-dioxacyclopropane	SEL(g)	43.9	3.0					1992DOR
$C_2H_4O_2$	1,2-dioxacyclobutane	SEL(g)	77.0	4.0					1992DOR
$C_2H_4O_3$	1,2,3-trioxacyclopentane	SEL(g)	78.0	4.5					1992DOR
$C_3H_6O_2$	1,3-dioxacyclopentane	SEL(g)	71.0	4.0					1992DOR
		SEL(l)			121.71	1.19			2019DIK
$C_3H_6O_3$	1,3,5-trioxacyclohexane	SEL	82.36	0.82			113.08	1.37	2019DIK
$C_4H_8O_2$	1,3-dioxane	SEL	89.54	0.90	140.3	2.4			2019DIK
	1,4-dioxane	SEL(g)	92.25	0.92					2019DIK
		SEL(l)			149.65	0.7			1993GRO
Cycloketones									
$C_{10}H_{16}O$	*D*-camphor	SEL	191	13			246.29	0.24	2019DIK
$C_4H_2O_3$	2,5-furandione	SEL	84.6	5.3			119.24	0.17	2019DIK
Aromatic Alcohols									
C_6H_6O	phenol	SEL(g)	103.22						1978KUD
		SEL(s)					127.21		1975NIC
C_7H_8O	2-methylphenol	SEL(g)	127.30						1978KUD
		SEL(s)					154.56	1.00	1967AND
	3-methylphenol	SEL(g)	124.68						1978KUD
		SEL(l)			224.93	1.30			1967AND
	benzyl alcohol	SEL(g)	126.8	8.1					2019DIK
		SEL(l)			215.94	1.00			1975NIC
Aromatic Aldehydes									
C_7H_6O	benzaldehyde	SEL(g)	111.70	1.00					1975AMB
		SEL(l)			172.00				1975AMB2
Aromatic Carboxylic Acids									
$C_7H_6O_2$	benzoic acid	SEL(g)	124.0	7.9					2019DIK
		SEL(s)					147.78	1.00	1993KAJ

Table 5-3(5). Nitrogen-Substituted Hydrocarbons

Formula	Compound	SEL	Cp(g)	U(Cpg) J mol-1 K-1	Cp(l)	U(Cpl)	Cp(s)	U(Cps)	Reference
Hydrogen Cyanides									
CHN	hydrogen cyanide	SEL	35.86	0.36	72.95	1.43			2019DIK
Alkyl Amines									
CH_5N	methylamine	SEL	50.08	0.50	104.8	2.7			2019DIK
C_2H_7N	ethylamine	SEL(g)	71.65	0.72					2019DIK
C_2H_7N	ethylamine	SEL(l)			129.5	4.8			2012KRO
C_3H_9N	1-propylamine	SEL(g)	91.25	0.91					2019DIK
		SEL(l)			162.51	1.00			1972FIN
	isopropylamine	SEL(g)	97.62	0.98					2019DIK
		SEL(l)							1972FIN
$C_4H_{11}N$	isobutylamine	SEL(g)	117.1	7.5					2019DIK
		SEL(l)			194.00				1971KON
	n-butylamine	SEL(g)	118.52	1.19					2019DIK
		SEL(l)			188.00	4.0			1971KON
	tert-butylamine	SEL(g)	121.00	1.21					2019DIK
		SEL(l)			190.00	1.0			1971KON
C_2H_7N	dimethylamine	SEL	70.45	0.70	140.5	2.6			2019DIK
C_3H_9N	methylethylamine	SEL	87.6	5.7					2019DIK
$C_4H_{11}N$	diethylamine	SEL(g)	115.77	1.16					2019DIK
		SEL(l)			178.10	0.8			1985COS
C_3H_9N	trimethylamine	SEL	91.80	0.92	138.15	0.99			2019DIK
$C_6H_{15}N$	*n*-hexylamine	SEL(g)	164	10					2019DIK
		SEL(l)			252.00	2.0			1971KON
	triethylamine	SEL(g)	160.98	1.61					2019DIK
		SEL(l)			216.43	2.0			1993GRO
$C_6H_{13}N$	cyclohexylamine	SEL	132.0	8.7	201.2	8.9			2019DIK
$C_6H_{12}N_4$	methenamine	SEL(s)					152.31	0.55	2019DIK
Alkanenitriles									
C_2H_3N	ethanenitrile	SEL	52.25	0.52	91.22	0.37			2019DIK
C_3H_5N	propanenitrile	SEL	73.77	0.74	120.26	0.89			2019DIK
C_4H_7N	butanenitrile	SEL	94.51	0.95	133.50	1.88			2019DIK
C_3H_3N	propenenitrile	SEL	63.93	0.64	108.48	0.49			2019DIK
Cyanogens									

C_2N_2	cyanogen	SEL	56.92	0.57	113.9	4.7			2019DIK
Hydrazines									
$C_2H_8N_2$	1,1-dimethylhydrazine	SEL	89.7	5.7	164.06	0.67			2019DIK
Aromatic Amines									
$C_3H_6N_6$	melamine	SEL	137.8	8.5			155.16	0.75	2019DIK
C_6H_7N	aniline	SEL(g)	108.14	1.08					2019DIK
		SEL(l)			191.01	1.20			1975NIC
$C_8H_{11}N$	*N*,*N*-dimethylaniline	SEL	151.2	9.8	211.9	5.6			2019DIK
Ureas									
CH_4N_2O	urea	SEL	77.55	0.78			92.79	0.32	2019DIK
Oxyamines									
$C_6H_{15}NO_3$	triethanolamine	SEL	213	13	361	21			2019DIK
Nitrates and Nitrites									
CH_3NO_3	methyl nitrate	SEL(g)	76.49	0.77					2019DIK
		SEL(l)			157.19				1953GRA
$C_3H_5N_3O_9$	nitroglycerin	SEL	234.5	2.6					2019DIK
CN_4O_8	tetranitromethane	SEL	171.6	5.4	207	11			2019DIK
CHN_3O_6	trinitromethane	SEL	131.5	3.8	182	11			2019DIK
CH_3NO_2	nitromethane	SEL(g)	57.27	0.57	106.25	0.78			2019DIK
		SEL(l)			105.98				1947JON
Isocyano Aromatics									
$C_9H_6N_2O_2$	2,4-diisocyanatotoluene	SEL			287.80				2019DIK
Nitro Aromatics									
$C_6H_3N_3O_6$	trinitrobenzene	SEL(g)	197.48	1.97					2019DIK
		SEL(s)					215	5	1980RAD
$C_6H_5NO_2$	nitrobenzene	SEL(g)	119.57	1.20					2019DIK
		SEL(l)			181.13	2.0			1985LAI
$C_7H_5N_3O_6$	trinitrotoluene	SEL(g)	213.3	5.6					2019DIK
		SEL(s)					243	10	1991YIN

Table 5-3(6). Sulfur-Substituted Hydrocarbons

Formula	Compound	SEL	C_p(g)	$U(C_p g)$ J mol^{-1} K^{-1}	C_p(l)	$U(C_p l)$	C_p(s)	$U(C_p s)$	Reference
Alkanethiols									
CH_4S	methanethiol	SEL	50.31	0.50	90.47	0.63			2019DIK
C_2H_6S	ethanethiol	SEL(g)	73.02	0.73					2019DIK
		SEL(l)			117.99	0.2			1952MCC
Alkyl Sulfides									
CS_2	carbon disulfide	SEL(g)	45.51	0.46					2019DIK
		SEL(l)			78.99	0.80			1955STA
C_2H_6S	dimethyl sulfide	SEL	74.08	0.74	118.28	0.84			2019DIK
C_2H_6OS	dimethyl sulfoxide	SEL(g)	89.43	0.89					2019DIK
		SEL(l)			149.39	1.0			1993GRO

Table 5-3(7). Halogenated Hydrocarbons

Formula	Compound	SEL	C_p(g)	$U(C_p g)$ J mol^{-1} K^{-1}	C_p(l)	$U(C_p l)$	C_p(s)	$U(C_p s)$	Reference
Fluoroalkanes									
CH_3F	fluoromethane	SEL(g)	37.49						1998CHA
		SEL(l)			106.26	1.09			1998HO
CH_2F_2	difluoromethane	SEL(g)	42.83						1998CHA
		SEL(l)			97.26	0.80			1996LUD
CHF_3	trifluoromethane	SEL	51.04	0.30					1962VAL
CF_4	tetrafluoromethane	SEL	61.02						1998CHA
C_2H_5F	fluoroethane	SEL	59.62	0.60	108.9	2.2			2018LEM
$C_2H_4F_2$	1,1-difluoroethane	SEL	67.48	0.67	118.9	1.2			2018LEM
$C_2H_4F_2$	1,2-difluoroethane	SEL	67.77	0.68	217.0	7.2			2019DIK
$C_2H_3F_3$	1,1,1-trifluoroethane	SEL	78.08	0.16	140.24	0.70			2018LEM
	1,1,2-trifluoroethane	SEL	77.42	0.77	137.5	4.6			2019DIK
$C_2H_2F_4$	1,1,1,2-tetrafluoroethane	SEL	85.03	0.21	145.36	0.73			2019DIK
	1,1,2,2-tetrafluoroethane	SEL	90.35	0.90	147.7	5.8			2019DIK
C_2HF_5	pentafluoroethane	SEL	94.44	0.94	166.0	6.7			2019DIK
C_2F_6	hexafluoroethane	SEL	106.61	1.07					2019DIK
Fluoroalkenes									
C_2H_3F	fluoroethene	SEL	50.43	0.50	99.1	6.7			2019DIK
$C_2H_2F_2$	1,1-difluoroethene	SEL	59.08	0.59					2019DIK
	1,2-difluoroethene, (E)-	SEL	60.26	0.60	129.9	8.0			2019DIK
	1,2-difluoroethene, (Z)-	SEL	58.35	0.58	103.5	5.5			2019DIK
C_2HF_3	trifluoroethene	SEL	69.20	0.69	145	11			2019DIK
C_2F_4	tetrafluoroethene	SEL	80.42	0.80					2019DIK
Chloroalkanes									
CH_3Cl	chloromethane	SEL(g)	40.74	0.41					2019DIK
		SEL(l)			81.70	0.50			1940AWB
CH_2Cl_2	dichloromethane	SEL(g)	50.85						1998CHA
		SEL(l)			98.6	2.4			2015CHO
$CHCl_3$	trichloromethane	SEL(g)	65.33						1998CHA
		SEL(l)			113.20				1993SHE
CCl_4	tetrachloromethane	SEL(g)	82.65						1998CHA
		SEL(l)			131.34				1982TAN
C_2H_5Cl	chloroethane	SEL	62.65	0.63	105.31	0.81			2019DIK

$C_2H_4Cl_2$	1,1-dichloroethane	SEL	76.33	0.76	126.44	0.63			2019DIK
	1,2-dichloroethane	SEL	77.32	0.77	129.19	0.52			2019DIK
$C_2H_3Cl_3$	1,1,1-trichloroethane	SEL	92.33	0.92	144.37	0.81			2019DIK
	1,1,2-trichloroethane	SEL	84.94	0.85	141.4	5.1			2019DIK
$C_2H_2Cl_4$	1,1,1,2-tetrachloroethane	SEL	102.88	1.03	157.9	6.1			2019DIK
	1,1,2,2-tetrachloroethane	SEL(g)	98.97	0.99					2019DIK
		SEL(l)			168.00	1.5			1989WIL
C_2HCl_5	pentachloroethane	SEL	118.07	1.18	174.3	7.2			2019DIK
C_2Cl_6	hexachloroethane	SEL	136.78	1.37			198.24	1.64	2019DIK
Chloroalkenes									
C_2H_3Cl	chloroethene	SEL	53.60	0.54	96.2	3.3			2019DIK
$C_2H_2Cl_2$	1,1-dichloroethene	SEL	66.93	0.67	110.80	0.67			2019DIK
	1,2-dichloroethene, (E)-	SEL	66.55	0.67	113.83	1.18			2019DIK
	1,2-dichloroethene, (Z)-	SEL	65.00	0.65	112.85	1.12			2019DIK
C_2HCl_3	trichloroethene	SEL	79.75	1.00	128.70	1.13			2019DIK
C_2Cl_4	tetrachloroethene	SEL(g)	95.51						1993GRO
		SEL(l)			147.16				1989WIL
Chloroalkynes									
C_2HCl	chloroethyne	SEL	51.6	2.8	135.5	4.4			2019DIK
C_2Cl_2	dichloroethyne	SEL	61.1	3.2	185.1	8.0			2019DIK
Chloro Aromatic									
C_6H_5Cl	chlorobenzene	SEL(g)	97.99	0.98					2019DIK
		SEL(l)			152.10	1.1			1993SHE
Bromoalkanes									
CH_3Br	bromomethane	SEL	42.45	0.43	81.59	1.21			2019DIK
CH_2Br_2	dibromomethane	SEL(g)	54.59	0.55	104.48	0.88			2019DIK
		SEL(l)			104.1	3.1			1993SHE
$CHBr_3$	tribromomethane	SEL	70.99	0.71	121.5	6.3			2019DIK
CBr_4	tetrabromomethane	SEL(g)	90.71						1998CHA
		SEL(s)					145.90		1984BIC
C_2H_5Br	bromoethane	SEL(g)	64.27	0.64					2019DIK
		SEL(l)			105.80	1.0			1993SHE
C_2H_3Br	bromoethene	SEL(g)	55.49	0.56					2019DIK
		SEL(l)			114.3	3.7			2012KRO
Iodoalkanes									
CH_3I	iodomethane	SEL(g)	44.08	0.44	82.58	0.61			2019DIK
		SEL(l)			82.75				1993CAR

CH_2I_2	diiodomethane	SEL(g)	57.75	0.58			2019DIK
		SEL(l)			112.80	6.0	1993SHE
CHI_3	triiodomethane	SEL(g)	75.06	0.75			2019DIK
		SEL(l)			157.50		1993CAR
CI_4	tetraiodomethane	SEL(g)	95.78	0.96			2019DIK
		SEL(l)			259.80		1993CAR
Chlorofluoroalkanes							
CH_2ClF	chlorofluoromethane	SEL(g)	47.29	0.46			1965BAR
		SEL(l)	47.08	0.47	73.2	2.4	2019DIK
$CHCl_2F$	dichlorofluoromethane	SEL(g)	61.33	0.64			1965BAR
		SEL(l)			107.5	3.8	2019DIK
$CHClF_2$	chlorodifluoromethane	SEL(g)	56.00	0.22			1995ESP
		SEL(l)			107.2	3.2	1940BEN
CCl_2F_2	dichlorodifluoromethane	SEL(g)	73.92	0.21			1991BUF
		SEL(l)			119.9	4.8	2019DIK
CCl_3F	trichlorofluoromethane	SEL(g)	78.09	0.78			2019DIK
		SEL(l)			121.55	0.46	1941OSB
$CClF_3$	chlorotrifluoromethane	SEL	66.87	0.67			2019DIK
C_2ClF_3	chlorotrifluoroethene	SEL	83.94	0.84	137.0	2.7	2019DIK
Bromofluoroalkanes							
CH_2BrF	bromofluoromethane	SEL	49.14	0.49	114.3	3.8	2019DIK
$CHBrF_2$	bromodifluoromethane	SEL	58.78	0.59	106.5	3.8	2019DIK
CBr_2F_2	dibromodifluoromethane	SEL	77.02	0.77	118.6	3.6	2019DIK
CBr_3F	tribromofluoromethane	SEL	84.37	0.84	169.7	6.4	2019DIK
$CBrF_3$	bromotrifluoromethane	SEL	69.26	0.69	125.24	0.27	2019DIK
Bromochloroalkanes							
CH_2BrCl	bromochloromethane	SEL(g)	52.76	0.53			2019DIK
		SEL(l)			104.1	1.5	2015CHO
$CHBr_2Cl$	dibromochloromethane	SEL	69.15	0.69	129.3	5.2	2019DIK
$CHBrCl_2$	bromodichloromethane	SEL	67.25	0.67	115.9	3.6	2019DIK
CBr_2Cl_2	dibromodichloromethane	SEL	87.15	0.87	140.43	1.08	2019DIK
$CBrCl_3$	bromotrichloromethane	SEL	85.38	0.85	135.29	0.56	2019DIK
Bromochlorofluoroalkanes							
CHBrClF	bromochlorofluoromethane	SEL	62.85	0.63	103.9	3.6	2019DIK
CBr_2ClF	dibromochlorofluoromethane	SEL	82.33	0.82	130.0	4.8	2019DIK
$CBrCl_2F$	bromodichlorofluoromethane	SEL	80.06	0.80	126.4	4.4	2019DIK
$CBrClF_2$	bromochlorodifluoromethane	SEL	74.66	0.75	118.8	3.9	2019DIK

Carbonyl Halides							
CCl_2O	phosgene	SEL(g)	57.69	0.58			1998CHA
		SEL(l)			104.08	0.97	2019DIK
Chloroaromatic Alcohols							
C_6HCl_5O	pentachlorophenol	SEL(g)	189.80	1.90			2019DIK
		SEL(l)			201.96		1958HIL
Siloxanes							
$C_6H_{18}OSi_2$	hexamethyldisiloxane	SEL			311.38	0.82	2019DIK
$C_8H_{24}O_4Si_4$	octamethylcyclotetrasiloxane	SEL			495.9	9.5	2019DIK

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