Propane, 1-methoxy-2,2-dimethyl-

Other names: Ether, methyl neopentyl
(CH3)3CCH2OCH3
Neopentyl methyl ether
Inchi: InChI=1S/C6H14O/c1-6(2,3)5-7-4/h5H2,1-4H3
InchiKey: JILHZKWLEAKYRC-UHFFFAOYSA-N
Formula: C6H14O
SMILES: COCC(C)(C)C
Mol. weight [g/mol]: 102.17
CAS: 1118-00-9

Physical Properties

Property code	Value	Unit	Source
affp	825.80	kJ/mol	NIST Webbook
basg	796.70	kJ/mol	NIST Webbook
gf	-102.52	kJ/mol	Joback Method
hf	-308.14	kJ/mol	Joback Method
hfus	5.07	kJ/mol	Joback Method
hvap	30.06	kJ/mol	Joback Method
ie	9.30 ± 0.05	eV	NIST Webbook
ie	9.64 ± 0.05	eV	NIST Webbook
ie	9.41	eV	NIST Webbook
log10ws	-1.18		Crippen Method
logp	1.679		Crippen Method
mcvol	101.270	ml/mol	McGowan Method
pc	3114.04	kPa	Joback Method
tb	355.87	K	Joback Method
tc	531.48	K	Joback Method
tf	182.03	K	Joback Method
vc	0.379	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	182.43	J/mol×K	355.87	Joback Method

cpg	194.11	J/mol×K	385.14	Joback Method
cpg	205.32	J/mol×K	414.41	Joback Method
cpg	216.07	J/mol×K	443.68	Joback Method
cpg	226.37	J/mol×K	472.94	Joback Method
cpg	236.25	J/mol×K	502.21	Joback Method
cpg	245.69	J/mol×K	531.48	Joback Method
dvisc	0.0072406	Pa×s	182.03	Joback Method
dvisc	0.0028457	Pa×s	211.00	Joback Method
dvisc	0.0014013	Pa×s	239.98	Joback Method
dvisc	0.0008039	Pa×s	268.95	Joback Method
dvisc	0.0005138	Pa×s	297.92	Joback Method
dvisc	0.0003555	Pa×s	326.90	Joback Method
dvisc	0.0002612	Pa×s	355.87	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1118009&Units=SI

Legend

affp: Proton affinity

basg: Gas basicity

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

gf: Standard Gibbs free energy of formation

hf: Enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

hvap: Enthalpy of vaporization at standard conditions

ie: Ionization energy

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

pc: Critical Pressure

tb: Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume