1-Methoxycyclohexane

Other names:	Ether, cyclohexyl methyl
	Cyclohexyl methyl ether
	Methoxycyclohexane
	Methyl cyclohexyl ether
	Cyclohexane, methoxy-
Inchi:	InChI=1S/C7H14O/c1-8-7-5-3-2-4-6-7/h7H,2-6H2,1H3
InchiKey:	GHDIHPNJQVDFBL-UHFFFAOYSA-N
Formula:	C7H14O
SMILES:	COC1CCCCC1
Mol. weight [g/mol]:	114.19
CAS:	931-56-6

Physical Properties

Property code	Value	Unit	Source
affp	840.50	kJ/mol	NIST Webbook
basg	811.30	kJ/mol	NIST Webbook
gf	-72.49	kJ/mol	Joback Method
hf	-265.71	kJ/mol	Joback Method
hfus	6.91	kJ/mol	Joback Method
hvap	34.02	kJ/mol	Joback Method
ie	9.22 ± 0.03	eV	NIST Webbook
log10ws	-1.85		Crippen Method
logp	1.965		Crippen Method
mcvol	104.500	ml/mol	McGowan Method
pc	3452.08	kPa	Joback Method
tb	403.15 ± 2.00	K	NIST Webbook
tb	406.60 ± 0.50	K	NIST Webbook
tc	603.65	K	Joback Method
tf	198.78 ± 0.30	K	NIST Webbook
vc	0.379	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	197.64	J/mol×K	401.53	Joback Method
cpg	213.41	J/mol×K	435.22	Joback Method
cpg	228.53	J/mol×K	468.90	Joback Method
cpg	242.98	J/mol×K	502.59	Joback Method
cpg	256.78	J/mol×K	536.27	Joback Method
cpg	269.94	J/mol×K	569.96	Joback Method
cpg	282.47	J/mol×K	603.65	Joback Method
dvisc	0.0056551	Pa×s	198.26	Joback Method
dvisc	0.0023106	Pa×s	232.14	Joback Method
dvisc	0.0011858	Pa×s	266.02	Joback Method
dvisc	0.0007076	Pa×s	299.89	Joback Method
dvisc	0.0004689	Pa×s	333.77	Joback Method
dvisc	0.0003352	Pa×s	367.65	Joback Method
dvisc	0.0002536	Pa×s	401.53	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=C931566&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