1-Methoxycyclohexene

Other names:	Ether, 1-cyclohexen-1-yl methyl
	Cyclohexanone methyl enol ether
	1-Cyclohexen-1-yl methyl ether
	1-Methoxy-1-cyclohexene
	1-Methoxycyclohexene
	2,3,4,5-Tetrahydroanisole
Inchi:	InChI=1S/C7H12O/c1-8-7-5-3-2-4-6-7/h5H,2-4,6H2,1H3
InchiKey:	HZFQGYWRFABYSR-UHFFFAOYSA-N
Formula:	C7H12O
SMILES:	COC1=CCCCC1
Mol. weight [g/mol]:	112.17

Physical Properties

Property code	Value	Unit	Source
hf	-161.00	kJ/mol	NIST Webbook
hfus	6.67	kJ/mol	Joback Method
hvap	43.70 ± 0.20	kJ/mol	NIST Webbook
ie	8.18	eV	Cheméo Relay (1.0)
log10ws	-1.92		Cheméo Relay (1.0)
logp	2.091		Crippen Method
mcvol	100.200	ml/mol	McGowan Method
pc	3682.02	kPa	Joback Method
rinpol	1014.00		NIST Webbook
rinpol	1014.00		NIST Webbook
tb	423.08	K	Cheméo Relay (1.0)
tc	620.22	K	Cheméo Relay (1.0)
tf	199.29	K	Cheméo Relay (1.0)
vc	0.345	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.07	J/mol×K	410.34	Joback Method
cpg	259.42	J/mol×K	616.67	Joback Method

cpg	248.66	J/mol×K	582.29	Joback Method
cpg	237.32	J/mol×K	547.90	Joback Method
cpg	225.40	J/mol×K	513.51	Joback Method
cpg	212.89	J/mol×K	479.12	Joback Method
cpg	199.79	J/mol×K	444.73	Joback Method
dvisc	0.0006340	Pa×s	313.06	Joback Method
dvisc	0.0002339	Pa×s	410.34	Joback Method
dvisc	0.0003081	Pa×s	377.91	Joback Method
dvisc	0.0004273	Pa×s	345.49	Joback Method
dvisc	0.0042221	Pa×s	215.78	Joback Method
dvisc	0.0010307	Pa×s	280.63	Joback Method
dvisc	0.0019026	Pa×s	248.21	Joback Method
hvapt	44.00 ± 0.20	kJ/mol	293.50	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C931577&Units=SI

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

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

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

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

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices

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