

Cyclohexene, 1-methoxy-

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
CAS:	931-57-7

Physical Properties

Property code	Value	Unit	Source
gf	-44.45	kJ/mol	Joback Method
hf	-161.00	kJ/mol	NIST Webbook
hfus	6.67	kJ/mol	Joback Method
hvap	43.70 ± 0.20	kJ/mol	NIST Webbook
log10ws	-2.08		Crippen Method
logp	2.091		Crippen Method
mvol	100.200	ml/mol	McGowan Method
pc	3682.02	kPa	Joback Method
rinpol	1014.00		NIST Webbook
rinpol	1014.00		NIST Webbook
tb	410.34	K	Joback Method
tc	616.67	K	Joback Method
tf	215.78	K	Joback Method
vc	0.365	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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
cpg	186.07	J/mol×K	410.34	Joback Method
dvisc	0.0042221	Paxs	215.78	Joback Method
dvisc	0.0002339	Paxs	410.34	Joback Method
dvisc	0.0003081	Paxs	377.91	Joback Method
dvisc	0.0004273	Paxs	345.49	Joback Method
dvisc	0.0006340	Paxs	313.06	Joback Method
dvisc	0.0010307	Paxs	280.63	Joback Method
dvisc	0.0019026	Paxs	248.21	Joback Method
hvapt	44.00 ± 0.20	kJ/mol	293.50	NIST Webbook

Sources

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=C931577&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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
hvapt:	Enthalpy of vaporization at a given temperature
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

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