

1-Cyclohexene-1-methanol

Other names:	1-Hydroxymethylcyclohexene 3-Methoxycyclohexene 3-Methoxycyclohexene-1 1-Cyclohexen-1-methanol
Inchi:	InChI=1S/C7H12O/c8-6-7-4-2-1-3-5-7/h4,8H,1-3,5-6H2
InchiKey:	QBJOHGAEIAUULA-UHFFFAOYSA-N
Formula:	C7H12O
SMILES:	OCC1=CCCCC1
Mol. weight [g/mol]:	112.17
CAS:	4845-04-9

Physical Properties

Property code	Value	Unit	Source
gf	-76.27	kJ/mol	Joback Method
hf	-219.07	kJ/mol	Joback Method
hfus	9.57	kJ/mol	Joback Method
hvap	49.55	kJ/mol	Joback Method
log10ws	-1.76		Crippen Method
logp	1.479		Crippen Method
mcvol	100.200	ml/mol	McGowan Method
pc	4222.04	kPa	Joback Method
tb	480.10	K	Joback Method
tc	676.31	K	Joback Method
tf	254.37	K	Joback Method
vc	0.366	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	214.26	J/mol×K	480.10	Joback Method
cpg	268.44	J/mol×K	643.61	Joback Method
cpg	258.77	J/mol×K	610.91	Joback Method
cpg	248.54	J/mol×K	578.21	Joback Method
cpg	237.72	J/mol×K	545.50	Joback Method

cpg	226.30	J/mol×K	512.80	Joback Method
cpg	277.57	J/mol×K	676.31	Joback Method
dvisc	0.0001751	Pa×s	480.10	Joback Method
dvisc	0.0002934	Pa×s	442.48	Joback Method
dvisc	0.0005410	Pa×s	404.86	Joback Method
dvisc	0.0011309	Pa×s	367.24	Joback Method
dvisc	0.0027975	Pa×s	329.61	Joback Method
dvisc	0.0087393	Pa×s	291.99	Joback Method
dvisc	0.0382405	Pa×s	254.37	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=C4845049&Units=SI

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
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

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