

3-Cyclohexene-1-methanol

Other names:	3-Cyclohexene-1-carbinol 4-(Hydroxymethyl)cyclohexene 1,2,3,6-Tetrahydrobenzyl alcohol 1-Hydroxymethyl-3-cyclohexene Cyclohex-3-en-1-ylmethanol 3-Cyclohexen-1-methanol cyclohex-3-ene-1-methanol
Inchi:	InChI=1S/C7H12O/c8-6-7-4-2-1-3-5-7/h1-2,7-8H,3-6H2
InchiKey:	VEIYJWQZNGASMA-UHFFFAOYSA-N
Formula:	C7H12O
SMILES:	OCC1CC=CCC1
Mol. weight [g/mol]:	112.17
CAS:	1679-51-2

Physical Properties

Property code	Value	Unit	Source
gf	-74.35	kJ/mol	Joback Method
hf	-227.94	kJ/mol	Joback Method
hfus	11.03	kJ/mol	Joback Method
hvap	48.58	kJ/mol	Joback Method
log10ws	-1.52		Crippen Method
logp	1.335		Crippen Method
mvol	100.200	ml/mol	McGowan Method
pc	4124.99	kPa	Joback Method
rinpol	1106.00		NIST Webbook
rinpol	1106.00		NIST Webbook
ripol	1696.00		NIST Webbook
ripol	1791.00		NIST Webbook
tb	470.45	K	Joback Method
tc	665.12	K	Joback Method
tf	237.61	K	Joback Method
vc	0.365	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	214.83	J/molxK	470.45	Joback Method
cpg	227.60	J/molxK	502.90	Joback Method
cpg	239.70	J/molxK	535.34	Joback Method
cpg	251.18	J/molxK	567.79	Joback Method
cpg	262.03	J/molxK	600.23	Joback Method
cpg	272.29	J/molxK	632.68	Joback Method
cpg	281.98	J/molxK	665.12	Joback Method
dvisc	0.0579900	Paxs	237.61	Joback Method
dvisc	0.0116411	Paxs	276.42	Joback Method
dvisc	0.0034700	Paxs	315.22	Joback Method
dvisc	0.0013487	Paxs	354.03	Joback Method
dvisc	0.0006318	Paxs	392.84	Joback Method
dvisc	0.0003392	Paxs	431.64	Joback Method
dvisc	0.0002018	Paxs	470.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1679512&Units=SI
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

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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