

3-Cyclohexen-1-ol

Other names:	Cyclohex-1-en-4-ol Cyclohexen-4-ol 3-Cyclohexenol 4-Hydroxycyclohexene Cyclohex-3-en-1-ol 3-Cyclohexene-1-ol
Inchi:	InChI=1S/C6H10O/c7-6-4-2-1-3-5-6/h1-2,6-7H,3-5H2
InchiKey:	ABZZOPIABWYXSN-UHFFFAOYSA-N
Formula:	C6H10O
SMILES:	OC1CC=CCC1
Mol. weight [g/mol]:	98.14
CAS:	822-66-2

Physical Properties

Property code	Value	Unit	Source
gf	-82.77	kJ/mol	Joback Method
hf	-207.30	kJ/mol	Joback Method
hfus	8.44	kJ/mol	Joback Method
hvap	46.35	kJ/mol	Joback Method
log10ws	-1.46		Crippen Method
logp	1.087		Crippen Method
mcvol	86.110	ml/mol	McGowan Method
pc	4684.89	kPa	Joback Method
rinpola	1097.00		NIST Webbook
tb	447.57	K	Joback Method
tc	644.50	K	Joback Method
tf	226.34	K	Joback Method
vc	0.309	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	173.65	J/mol×K	447.57	Joback Method
cpg	185.32	J/mol×K	480.39	Joback Method

cpg	196.39	J/molxK	513.21	Joback Method
cpg	206.87	J/molxK	546.03	Joback Method
cpg	216.79	J/molxK	578.86	Joback Method
cpg	226.15	J/molxK	611.68	Joback Method
cpg	234.98	J/molxK	644.50	Joback Method
dvisc	0.0721805	Paxs	226.34	Joback Method
dvisc	0.0142316	Paxs	263.21	Joback Method
dvisc	0.0041819	Paxs	300.08	Joback Method
dvisc	0.0016066	Paxs	336.95	Joback Method
dvisc	0.0007454	Paxs	373.83	Joback Method
dvisc	0.0003970	Paxs	410.70	Joback Method
dvisc	0.0002345	Paxs	447.57	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C822662&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
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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