1,3-Cyclohexanediol

Other names:	Resorcitol
	1,3-Benzenediol, hexahydro-
	1,3-Dihydroxycyclohexane
	1,3-Cyclohexanediol,c&t
	1,3-Cyclohexanediol cis+trans
	1,3-Cyclohexanediol cis-trans
	cyclohexane-1,3-diol
Inchi:	InChI=1S/C6H12O2/c7-5-2-1-3-6(8)4-5/h5-8H,1-4H2
InchiKey:	RLMGYIOTPQVQJR-UHFFFAOYSA-N
Formula:	C6H12O2
SMILES:	OC1CCCC(O)C1
Mol. weight [g/mol]:	116.16
CAS:	504-01-8

Physical Properties

Property code	Value	Unit	Source
gf	-257.26	kJ/mol	Joback Method
hf	-437.65	kJ/mol	Joback Method
hfus	12.38	kJ/mol	Joback Method
hvap	62.43	kJ/mol	Joback Method
log10ws	-0.98		Crippen Method
logp	0.282		Crippen Method
mcvol	96.280	ml/mol	McGowan Method
pc	4835.95	kPa	Joback Method
rinpol	1108.00		NIST Webbook
rinpol	1089.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1089.00		NIST Webbook
rinpol	1089.00		NIST Webbook
ripol	2070.00		NIST Webbook
tb	519.70	K	NIST Webbook
tc	720.36	K	Joback Method
tf	282.16	K	Joback Method
vc	0.342	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.23	J/mol×K	535.92	Joback Method
cpg	252.43	J/mol×K	566.66	Joback Method
cpg	263.09	J/mol×K	597.40	Joback Method
cpg	273.22	J/mol×K	628.14	Joback Method
cpg	282.84	J/mol×K	658.88	Joback Method
cpg	291.95	J/mol×K	689.62	Joback Method
cpg	300.56	J/mol×K	720.36	Joback Method
dvisc	0.0909733	Pa×s	282.16	Joback Method
dvisc	0.0131225	Pa×s	324.45	Joback Method
dvisc	0.0029585	Pa×s	366.75	Joback Method
dvisc	0.0009076	Pa×s	409.04	Joback Method
dvisc	0.0003475	Pa×s	451.33	Joback Method
dvisc	0.0001568	Pa×s	493.63	Joback Method
dvisc	0.0000802	Pa×s	535.92	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C504018&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