1,3-Cyclohexanediol, cis-

Other names: cis-1,3-Cyclohexanediol
1,3-Cyclohexanediol, (Z)-
cis-1,3-Cyclohexandiol
Inchi: InChI=1S/C6H12O2/c7-5-2-1-3-6(8)4-5/h5-8H,1-4H2/t5-,6+
InchiKey: RLMGYIOTPQVQJR-OLQVQODUSA-N
Formula: C6H12O2
SMILES: OC1CCCC(O)C1
Mol. weight [g/mol]: 116.16
CAS: 823-18-7

Physical Properties

Property code	Value	Unit	Source
affp	882.20	kJ/mol	NIST Webbook
basg	849.70	kJ/mol	NIST Webbook
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
tb	535.92	K	Joback Method
tc	720.36	K	Joback Method
tf	338.15 ± 2.00	K	NIST Webbook
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	291.95	J/mol×K	689.62	Joback Method
cpg	282.84	J/mol×K	658.88	Joback Method
cpg	273.22	J/mol×K	628.14	Joback Method

cpg	263.09	J/mol×K	597.40	Joback Method
cpg	252.43	J/mol×K	566.66	Joback Method
cpg	300.56	J/mol×K	720.36	Joback Method
dvisc	0.0000802	Pa×s	535.92	Joback Method
dvisc	0.0001568	Pa×s	493.63	Joback Method
dvisc	0.0003475	Pa×s	451.33	Joback Method
dvisc	0.0009076	Pa×s	409.04	Joback Method
dvisc	0.0029585	Pa×s	366.75	Joback Method
dvisc	0.0131225	Pa×s	324.45	Joback Method
dvisc	0.0909733	Pa×s	282.16	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C823187&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

affp: Proton affinity
basg: Gas basicity
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