CIS-1,5-CYCLOOCTANEDIOL

Other names: 1,5-Cyclooctanediol, cis-
cis-cyclooctane-1,5-diol
Inchi: InChI=1S/C8H16O2/c9-7-3-1-4-8(10)6-2-5-7/h7-10H,1-6H2/t7-,8+
InchiKey: BDNXUVOJBGHQFD-OCAPTIKFSA-N
Formula: C8H16O2
SMILES: O[C@H]1CCC[C@@H](O)CCC1
Mol. weight [g/mol]: 144.21

Physical Properties

Property code	Value	Unit	Source
af	0.5919		Cheméo Relay (1.0)
gf	-264.62	kJ/mol	Joback Method
hf	-466.97	kJ/mol	Cheméo Relay (1.0)
hfus	13.36	kJ/mol	Joback Method
hvap	95.82	kJ/mol	Cheméo Relay (1.0)
ie	9.76	eV	Cheméo Relay (1.0)
log10ws	-1.16		Cheméo Relay (1.0)
logp	1.062		Crippen Method
mcvol	124.460	ml/mol	McGowan Method
pc	4005.77	kPa	Joback Method
tb	535.73	K	Cheméo Relay (1.0)
tc	751.59	K	Cheméo Relay (1.0)
tf	355.60	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.42	J/mol×K	590.22	Joback Method
cpg	411.02	J/mol×K	782.42	Joback Method
cpg	400.39	J/mol×K	750.38	Joback Method
cpg	389.05	J/mol×K	718.35	Joback Method
cpg	376.98	J/mol×K	686.32	Joback Method
cpg	364.19	J/mol×K	654.29	Joback Method
cpg	350.68	J/mol×K	622.25	Joback Method

dvisc	0.0004079	Pa×s	443.94	Joback Method
dvisc	0.0000279	Pa×s	590.22	Joback Method
dvisc	0.0000580	Pa×s	541.46	Joback Method
dvisc	0.0001397	Pa×s	492.70	Joback Method
dvisc	0.0834069	Pa×s	297.66	Joback Method
dvisc	0.0015514	Pa×s	395.18	Joback Method
dvisc	0.0085936	Pa×s	346.42	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23418828&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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