

1,2-Cyclooctanediol, (E)-

Other names:	1,2-Cyclooctanediol, (E)- trans-cyclooctane-1,2-diol
Inchi:	InChI=1S/C8H16O2/c9-7-5-3-1-2-4-6-8(7)10/h7-10H,1-6H2
InchiKey:	HUSOFJYAGDTKSK-UHFFFAOYSA-N
Formula:	C8H16O2
SMILES:	OC1CCCCCCC1O
Mol. weight [g/mol]:	144.21

Physical Properties

Property code	Value	Unit	Source
af	0.6063		Cheméo Relay (1.0)
gf	-264.62	kJ/mol	Joback Method
hf	-457.71	kJ/mol	Cheméo Relay (1.0)
hfus	13.36	kJ/mol	Joback Method
hvap	92.79	kJ/mol	Cheméo Relay (1.0)
ie	9.70	eV	Cheméo Relay (1.0)
log10ws	-1.23		Cheméo Relay (1.0)
logp	1.062		Crippen Method
mcvol	124.460	ml/mol	McGowan Method
pc	4005.77	kPa	Joback Method
tb	528.06	K	Cheméo Relay (1.0)
tc	742.61	K	Cheméo Relay (1.0)
tf	380.11	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	350.68	J/mol×K	622.25	Joback Method
cpg	364.19	J/mol×K	654.29	Joback Method
cpg	376.98	J/mol×K	686.32	Joback Method
cpg	389.05	J/mol×K	718.35	Joback Method
cpg	400.39	J/mol×K	750.38	Joback Method
cpg	411.02	J/mol×K	782.42	Joback Method

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

Sources

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
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=C42565220&Units=SI

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

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