Loprodiol

Other names:	1,3-Propanediol, 2,2-bis(chloromethyl)-
	Chlorpropandiol
	Clorpropandiol
	Dispranol
	Gentimon
	Pentaerythritol dichlorohydrin
	2,2-Bis(chloromethyl)-1,3-propanediol
Inchi:	InChI=1S/C5H10Cl2O2/c6-1-5(2-7,3-8)4-9/h8-9H,1-4H2
InchiKey:	YFESJHPTNWYOCO-UHFFFAOYSA-N
Formula:	C5H10Cl2O2
SMILES:	OCC(CO)(CCl)CCl
Mol. weight [g/mol]:	173.04
CAS:	2209-86-1

Physical Properties

Property code	Value	Unit	Source
gf	-303.44	kJ/mol	Joback Method
hf	-491.22	kJ/mol	Joback Method
hfus	17.86	kJ/mol	Joback Method
hvap	67.56	kJ/mol	Joback Method
log10ws	-0.51		Crippen Method
logp	0.435		Crippen Method
mcvol	117.530	ml/mol	McGowan Method
pc	4062.13	kPa	Joback Method
rinpol	1340.00		NIST Webbook
tb	569.79	K	Joback Method
tc	746.34	K	Joback Method
tf	330.01	K	Joback Method
vc	0.441	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.07	J/mol×K	569.79	Joback Method

cpg	292.24	J/mol×K	716.92	Joback Method
cpg	286.73	J/mol×K	687.49	Joback Method
cpg	280.89	J/mol×K	658.07	Joback Method
cpg	274.68	J/mol×K	628.64	Joback Method
cpg	268.08	J/mol×K	599.22	Joback Method
cpg	297.43	J/mol×K	746.34	Joback Method
dvisc	0.0000528	Pa×s	569.79	Joback Method
dvisc	0.0000997	Pa×s	529.83	Joback Method
dvisc	0.0002089	Pa×s	489.86	Joback Method
dvisc	0.0004992	Pa×s	449.90	Joback Method
dvisc	0.0014137	Pa×s	409.94	Joback Method
dvisc	0.0050124	Pa×s	369.97	Joback Method
dvisc	0.0241478	Pa×s	330.01	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2209861&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume