1,2-Propanediol, 3-chloro-

Other names:	(.+/-.)-2,3-Dihydroxychloropropane
	.alpha.-chlorohydrin
	1,2-Dihydroxy-3-chloropropane
	1,2-Propanediol, 3-dichloro-
	1-Chloro-1-deoxyglycerol
	1-Chloro-2,3-dihydroxypropane
	1-Chloro-2,3-propanediol
	1-Chloropropane-2,3-diol
	2,3-Dihydroxypropyl chloride
	3-Chloro-1,2-dihydroxypropane
	3-Chloro-1,2-propandiol
	3-Chloro-1,2-propylene glycol
	3-Chloropropandiol-(1,2)
	3-Chloropropane-1,2-diol
	3-Chloropropanediol
	3-Chloropropylene glycol
	3-chloro-1,2-propanediol
	Chlorodeoxyglycerol
	Chloropropanediol
	Epibloc
	Glycerin epichlorohydrin
	Glycerin «alpha»-monochlorhydrin
	Glycerol 3-chlorohydrin
	Glycerol chlorohydrin
	Glycerol «alpha»-chlorohydrin
	Glycerol-«alpha»-monochlorohydrin
	Glyceryl chloride
	Glyceryl «alpha»-chlorohydrin
	U 5897
	UN 2689
	«alpha»-Chlorohydrin
	«alpha»-Monochlorohydrine
	«beta»,«beta»'-Dihydroxyisopropyl chloride
Inchi:	InChI=1S/C3H7ClO2/c4-1-3(6)2-5/h3,5-6H,1-2H2
InchiKey:	SSZWWUDQMAHNAQ-UHFFFAOYSA-N
Formula:	C3H7ClO2
SMILES:	OCC(O)CCl
Mol. weight [g/mol]:	110.54
CAS:	96-24-2

Physical Properties

Property code	Value	Unit	Source
chl	-1679.00 ± 0.40	kJ/mol	NIST Webbook
chl	-1683.51 ± 0.97	kJ/mol	NIST Webbook
gf	-313.63	kJ/mol	Joback Method
hf	-430.73	kJ/mol	Joback Method
hfl	-525.10 ± 0.80	kJ/mol	NIST Webbook
hfus	12.38	kJ/mol	Joback Method
hvap	59.63	kJ/mol	Joback Method
log10ws	0.13		Crippen Method
logp	-0.422		Crippen Method
mcvol	77.110	ml/mol	McGowan Method
pc	5478.85	kPa	Joback Method
tb	486.20	K	NIST Webbook
tc	657.67	K	Joback Method
tf	260.13	K	Joback Method
vc	0.284	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	183.12	J/mol×K	657.67	Joback Method
cpg	179.01	J/mol×K	629.63	Joback Method
cpg	174.69	J/mol×K	601.58	Joback Method
cpg	170.18	J/mol×K	573.53	Joback Method
cpg	165.45	J/mol×K	545.48	Joback Method
cpg	160.51	J/mol×K	517.44	Joback Method
cpg	155.35	J/mol×K	489.39	Joback Method
dvisc	0.2641302	Pa×s	260.13	Joback Method
dvisc	0.0001273	Pa×s	489.39	Joback Method
dvisc	0.0002651	Pa×s	451.18	Joback Method
dvisc	0.0006327	Pa×s	412.97	Joback Method
dvisc	0.0018028	Pa×s	374.76	Joback Method
dvisc	0.0065159	Pa×s	336.55	Joback Method
dvisc	0.0327290	Pa×s	298.34	Joback Method
hvapt	66.60	kJ/mol	376.00	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Interaction of some hydrophobic amino acids, peptides, and protein with aqueous 3-chloro-1,2-propanediol and 3-chloro-1-propanol: Biophysical studies.:	https://www.doi.org/10.1016/j.jct.2010.11.015
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C96242&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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