Chloral Hydrate

Other names:	1,1,1-Trichloro-2,2-dihydroxyethane
	1,1,1-Trichloro-2,2-ethanediol
	1,1-Ethanediol, 2,2,2-trichloro-
	2,2,2-Trichloro-1,1-ethanediol
	2,2,2-trichloroethane-1,1-diol
	Aquachloral
	Bi 3411
	Chloradorm
	Chloral monohydrate
	Chloraldurat
	Cohidrate
	Dormal
	Escre
	Felsules
	Hydral
	Hydrate de chloral
	Hynos
	Kessodrate
	Lorinal
	Lycoral
	NSC 3210
	Noctec
	Nortec
	Nycoton
	Nycton
	Oradrate
	Phaldrone
	Rectules
	SK-Chloral hydrate
	Somni Sed
	Somnos
	Sontec
	Tosyl
	Trawotox
	Trichloracetaldehyd-hydrat
	Trichloroacetaldehyde hydrate
	Trichloroacetaldehyde monohydrate
Inchi:	InChI=1S/C2H3Cl3O2/c3-2(4,5)1(6)7/h1,6-7H
InchiKey:	RNFNDJAIBTYOQL-UHFFFAOYSA-N
Formula:	C2H3Cl3O2

SMILES: OC(O)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 165.40
CAS: 302-17-0

Physical Properties

Property code	Value	Unit	Source
gf	-343.07	kJ/mol	Joback Method
hf	-450.32	kJ/mol	Joback Method
hfus	10.77	kJ/mol	Joback Method
hvap	64.88	kJ/mol	Joback Method
log10ws	0.72		Aqueous Solubility Prediction Method
log10ws	1.70		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	0.667		Crippen Method
mcvol	87.500	ml/mol	McGowan Method
pc	5827.17	kPa	Joback Method
rinpol	705.00		NIST Webbook
rinpol	698.00		NIST Webbook
rinpol	698.00		NIST Webbook
rinpol	695.00		NIST Webbook
tb	538.14	K	Joback Method
tc	728.62	K	Joback Method
tf	330.00 ± 15.00	K	NIST Webbook
tf	349.00 ± 3.00	K	NIST Webbook
vc	0.316	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	156.63	J/mol×K	538.14	Joback Method
cpg	160.16	J/mol×K	569.89	Joback Method
cpg	163.36	J/mol×K	601.63	Joback Method
cpg	166.26	J/mol×K	633.38	Joback Method
cpg	168.90	J/mol×K	665.13	Joback Method
cpg	171.29	J/mol×K	696.87	Joback Method
cpg	173.46	J/mol×K	728.62	Joback Method

dvisc	0.0026686	Pa×s	386.79	Joback Method
dvisc	0.0100500	Pa×s	348.96	Joback Method
dvisc	0.0522538	Pa×s	311.12	Joback Method
dvisc	0.0008975	Pa×s	424.63	Joback Method
dvisc	0.0003608	Pa×s	462.47	Joback Method
dvisc	0.0001664	Pa×s	500.30	Joback Method
dvisc	0.0000856	Pa×s	538.14	Joback Method
hsubt	50.90	kJ/mol	291.00	NIST Webbook
hvapt	38.40	kJ/mol	324.00	NIST Webbook
hvapt	49.60	kJ/mol	347.50	NIST Webbook
hvapt	51.50	kJ/mol	316.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C302170&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Aqueous and cosolvent solubility data for drug-like organic compounds: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/

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

hsubt: Enthalpy of sublimation at a given temperature

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

rinpol: Non-polar retention indices

tb: Normal Boiling Point Temperature

tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume