

chloralose

Other names:	1-[6-hydroxy-2-(trichloromethyl)-3a,5,6,6a-tetrahydrofuro[4,5-d][1,3]dioxol-5-yl]ethane-1,2
Inchi:	InChI=1S/C8H11Cl3O6/c9-8(10,11)7-16-5-3(14)4(2(13)1-12)15-6(5)17-7/h2-7,12-14H,1H
InchiKey:	OJYGBLRPYBAHRT-UHFFFAOYSA-N
Formula:	C8H11Cl3O6
SMILES:	OCC(O)C1OC2OC(C(Cl)(Cl)Cl)OC2C1O
Mol. weight [g/mol]:	309.53

Physical Properties

Property code	Value	Unit	Source
gf	-613.56	kJ/mol	Joback Method
hf	-1050.13	kJ/mol	Joback Method
hfus	49.61	kJ/mol	Joback Method
hvap	107.68	kJ/mol	Joback Method
log10ws	-1.84		Aqueous Solubility Prediction Method
log10ws	-1.84		Estimated Solubility Method
logp	-0.463		Crippen Method
mcvol	173.800	ml/mol	McGowan Method
pc	3857.88	kPa	Joback Method
tb	856.46	K	Joback Method
tc	1060.59	K	Joback Method
tf	535.39	K	Joback Method
vc	0.628	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.40	J/molxK	856.46	Joback Method
cpg	560.99	J/molxK	1026.57	Joback Method
cpg	555.15	J/molxK	992.55	Joback Method
cpg	548.92	J/molxK	958.52	Joback Method
cpg	542.26	J/molxK	924.50	Joback Method
cpg	535.11	J/molxK	890.48	Joback Method

cpg	566.52	J/mol×K	1060.59	Joback Method
dvisc	0.0000063	Paxs	856.46	Joback Method
dvisc	0.0000103	Paxs	802.95	Joback Method
dvisc	0.0000181	Paxs	749.44	Joback Method
dvisc	0.0000347	Paxs	695.92	Joback Method
dvisc	0.0000742	Paxs	642.41	Joback Method
dvisc	0.0001822	Paxs	588.90	Joback Method
dvisc	0.0005350	Paxs	535.39	Joback Method

Sources

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

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

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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