

Glycerine mono-alpha,alpha-dichloropropionate

Inchi:	InChI=1S/C6H10Cl2O4/c1-6(7,8)5(11)12-3-4(10)2-9/h4,9-10H,2-3H2,1H3
InchiKey:	MPXPHJHCZGNCNN-UHFFFAOYSA-N
Formula:	C6H10Cl2O4
SMILES:	CC(Cl)(Cl)C(=O)OCC(O)CO
Mol. weight [g/mol]:	217.05
CAS:	116402-61-0

Physical Properties

Property code	Value	Unit	Source
gf	-531.38	kJ/mol	Joback Method
hf	-761.94	kJ/mol	Joback Method
hfus	19.72	kJ/mol	Joback Method
hvap	78.55	kJ/mol	Joback Method
log10ws	-0.75		Crippen Method
logp	0.077		Crippen Method
mcvol	139.060	ml/mol	McGowan Method
pc	3853.09	kPa	Joback Method
tb	668.52	K	Joback Method
tc	853.65	K	Joback Method
tf	398.44	K	Joback Method
vc	0.514	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.33	J/molxK	668.52	Joback Method
cpg	367.48	J/molxK	822.79	Joback Method
cpg	362.05	J/molxK	791.94	Joback Method
cpg	356.23	J/molxK	761.08	Joback Method
cpg	350.02	J/molxK	730.23	Joback Method
cpg	343.39	J/molxK	699.37	Joback Method
cpg	372.56	J/molxK	853.65	Joback Method
dvisc	0.0000169	Paxs	668.52	Joback Method
dvisc	0.0000299	Paxs	623.51	Joback Method

dvisc	0.0000580	Paxs	578.49	Joback Method
dvisc	0.0001258	Paxs	533.48	Joback Method
dvisc	0.0003144	Paxs	488.47	Joback Method
dvisc	0.0009467	Paxs	443.45	Joback Method
dvisc	0.0036563	Paxs	398.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402610&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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