

Diglycolic acid, 2,3-dichlorophenyl propyl ester

Inchi:	InChI=1S/C13H14Cl2O5/c1-2-6-19-11(16)7-18-8-12(17)20-10-5-3-4-9(14)13(10)15/h3-5H
InchiKey:	KXDZFOXNMNCKKF-UHFFFAOYSA-N
Formula:	C13H14Cl2O5
SMILES:	CCCOC(=O)COCC(=O)Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]:	321.15

Physical Properties

Property code	Value	Unit	Source
gf	-444.97	kJ/mol	Joback Method
hf	-751.36	kJ/mol	Joback Method
hfus	37.84	kJ/mol	Joback Method
hvap	77.62	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.869		Crippen Method
mvol	215.500	ml/mol	McGowan Method
pc	2135.43	kPa	Joback Method
rinpol	2676.00		NIST Webbook
rinpol	2676.00		NIST Webbook
tb	783.34	K	Joback Method
tc	997.68	K	Joback Method
tf	514.12	K	Joback Method
vc	0.820	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	560.69	J/molxK	783.34	Joback Method
cpg	572.11	J/molxK	819.06	Joback Method
cpg	582.60	J/molxK	854.79	Joback Method
cpg	592.16	J/molxK	890.51	Joback Method
cpg	600.77	J/molxK	926.24	Joback Method
cpg	608.41	J/molxK	961.96	Joback Method
cpg	615.09	J/molxK	997.68	Joback Method
dvisc	0.0004934	Paxs	514.12	Joback Method

dvisc	0.0003254	Paxs	558.99	Joback Method
dvisc	0.0002283	Paxs	603.86	Joback Method
dvisc	0.0001682	Paxs	648.73	Joback Method
dvisc	0.0001289	Paxs	693.60	Joback Method
dvisc	0.0001021	Paxs	738.47	Joback Method
dvisc	0.0000830	Paxs	783.34	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382088&Units=SI
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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