Diglycolic acid, 2,3-dichlorophenyl ethyl ester

Inchi: InChI=1S/C12H12Cl2O5/c1-2-18-10(15)6-17-7-11(16)19-9-5-3-4-8(13)12(9)14/h3-5H,2,6
InchiKey: AOQJXIWCPYFGGN-UHFFFAOYSA-N
Formula: C12H12Cl2O5
SMILES: CCOC(=O)COCC(=O)Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]: 307.13

Physical Properties

Property code	Value	Unit	Source
gf	-453.39	kJ/mol	Joback Method
hf	-730.72	kJ/mol	Joback Method
hfus	35.25	kJ/mol	Joback Method
hvap	75.40	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	2.478		Crippen Method
mcvol	201.410	ml/mol	McGowan Method
pc	2338.29	kPa	Joback Method
rinpol	2558.00		NIST Webbook
rinpol	2558.00		NIST Webbook
tb	760.46	K	Joback Method
tc	977.36	K	Joback Method
tf	502.85	K	Joback Method
vc	0.763	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	507.79	J/mol×K	760.46	Joback Method
cpg	553.85	J/mol×K	941.21	Joback Method
cpg	546.45	J/mol×K	905.06	Joback Method
cpg	538.12	J/mol×K	868.91	Joback Method
cpg	528.89	J/mol×K	832.76	Joback Method
cpg	518.77	J/mol×K	796.61	Joback Method
cpg	560.32	J/mol×K	977.36	Joback Method
dvisc	0.0000948	Pa×s	760.46	Joback Method

dvisc	0.0001161	Pa×s	717.53	Joback Method
dvisc	0.0001458	Pa×s	674.59	Joback Method
dvisc	0.0001890	Pa×s	631.65	Joback Method
dvisc	0.0002543	Pa×s	588.72	Joback Method
dvisc	0.0003586	Pa×s	545.79	Joback Method
dvisc	0.0005363	Pa×s	502.85	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U382087&Units=SI

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