Diglycolic acid, 2,3-dichlorophenyl octyl ester

Inchi: InChI=1S/C18H24Cl2O5/c1-2-3-4-5-6-7-11-24-16(21)12-23-13-17(22)25-15-10-8-9-14(19
InchiKey: MPCPJOYEFVBHLN-UHFFFAOYSA-N
Formula: C18H24Cl2O5
SMILES: CCCCCCCCOC(=O)COCC(=O)Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]: 391.29

Physical Properties

Property code	Value	Unit	Source
gf	-402.87	kJ/mol	Joback Method
hf	-854.56	kJ/mol	Joback Method
hfus	50.79	kJ/mol	Joback Method
hvap	88.75	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	4.819		Crippen Method
mcvol	285.950	ml/mol	McGowan Method
pc	1430.46	kPa	Joback Method
rinpol	3311.00		NIST Webbook
rinpol	3311.00		NIST Webbook
tb	897.74	K	Joback Method
tc	1108.53	K	Joback Method
tf	570.47	K	Joback Method
vc	1.099	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	839.69	J/mol×K	897.74	Joback Method
cpg	891.46	J/mol×K	1073.39	Joback Method
cpg	883.48	J/mol×K	1038.26	Joback Method
cpg	874.31	J/mol×K	1003.13	Joback Method
cpg	863.96	J/mol×K	968.00	Joback Method
cpg	852.42	J/mol×K	932.87	Joback Method
cpg	898.27	J/mol×K	1108.53	Joback Method
dvisc	0.0000409	Pa×s	897.74	Joback Method

dvisc	0.0000513	Pa×s	843.19	Joback Method
dvisc	0.0000664	Pa×s	788.65	Joback Method
dvisc	0.0000892	Pa×s	734.11	Joback Method
dvisc	0.0001257	Pa×s	679.56	Joback Method
dvisc	0.0001881	Pa×s	625.01	Joback Method
dvisc	0.0003039	Pa×s	570.47	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=U382095&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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