Diglycolic acid, 2,3-dichlorophenyl hexyl ester

Inchi: InChI=1S/C16H20Cl2O5/c1-2-3-4-5-9-22-14(19)10-21-11-15(20)23-13-8-6-7-12(17)16(13
InchiKey: POKUFUFTSBWCLX-UHFFFAOYSA-N
Formula: C16H20Cl2O5
SMILES: CCCCCCOC(=O)COCC(=O)Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]: 363.23

Physical Properties

Property code	Value	Unit	Source
gf	-419.71	kJ/mol	Joback Method
hf	-813.28	kJ/mol	Joback Method
hfus	45.61	kJ/mol	Joback Method
hvap	84.30	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	4.039		Crippen Method
mcvol	257.770	ml/mol	McGowan Method
pc	1663.26	kPa	Joback Method
rinpol	3068.00		NIST Webbook
rinpol	3068.00		NIST Webbook
tb	851.98	K	Joback Method
tc	1062.16	K	Joback Method
tf	547.93	K	Joback Method
vc	0.988	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	725.51	J/mol×K	851.98	Joback Method
cpg	776.36	J/mol×K	1027.13	Joback Method
cpg	768.36	J/mol×K	992.10	Joback Method
cpg	759.27	J/mol×K	957.07	Joback Method
cpg	749.10	J/mol×K	922.04	Joback Method
cpg	737.85	J/mol×K	887.01	Joback Method
cpg	783.27	J/mol×K	1062.16	Joback Method
dvisc	0.0000547	Pa×s	851.98	Joback Method

dvisc	0.0000681	Pa×s	801.31	Joback Method
dvisc	0.0000873	Pa×s	750.63	Joback Method
dvisc	0.0001160	Pa×s	699.96	Joback Method
dvisc	0.0001612	Pa×s	649.28	Joback Method
dvisc	0.0002368	Pa×s	598.61	Joback Method
dvisc	0.0003735	Pa×s	547.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382093&Units=SI
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

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