Diglycolic acid, 2,3-dichlorophenyl isohexyl ester

Inchi: InChI=1S/C16H20Cl2O5/c1-11(2)5-4-8-22-14(19)9-21-10-15(20)23-13-7-3-6-12(17)16(13

InchiKey: BSJSIFBVBFFULB-UHFFFAOYSA-N

Formula: C16H20Cl2O5

SMILES: CC(C)CCCOC(=O)COCC(=O)Oc1cccc(Cl)c1Cl

Mol. weight [g/mol]: 363.23

Physical Properties

Property code	Value	Unit	Source
gf	-422.15	kJ/mol	Joback Method
hf	-818.56	kJ/mol	Joback Method
hfus	42.09	kJ/mol	Joback Method
hvap	83.91	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	3.895		Crippen Method
mcvol	257.770	ml/mol	McGowan Method
pc	1674.16	kPa	Joback Method
rinpol	3018.00		NIST Webbook
rinpol	3018.00		NIST Webbook
tb	851.54	K	Joback Method
tc	1064.03	K	Joback Method
tf	532.93	K	Joback Method
vc	0.982	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	726.08	J/mol×K	851.54	Joback Method
cpg	738.53	J/mol×K	886.96	Joback Method
cpg	749.86	J/mol×K	922.37	Joback Method
cpg	760.08	J/mol×K	957.79	Joback Method
cpg	769.18	J/mol×K	993.20	Joback Method
cpg	777.15	J/mol×K	1028.62	Joback Method
cpg	784.00	J/mol×K	1064.03	Joback Method
dvisc	0.0004081	Pa×s	532.93	Joback Method

dvisc	0.0002456	Pa×s	586.03	Joback Method
dvisc	0.0001608	Pa×s	639.13	Joback Method
dvisc	0.0001123	Pa×s	692.24	Joback Method
dvisc	0.0000826	Pa×s	745.34	Joback Method
dvisc	0.0000633	Pa×s	798.44	Joback Method
dvisc	0.0000501	Pa×s	851.54	Joback Method

Sources

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=U382092&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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