

Diglycolic acid, 2,6-dichlorophenyl isohexyl ester

Inchi:	InChI=1S/C16H20Cl2O5/c1-11(2)5-4-8-22-14(19)9-21-10-15(20)23-16-12(17)6-3-7-13(18)
InchiKey:	VGEBJKUCDIFHTQ-UHFFFAOYSA-N
Formula:	C16H20Cl2O5
SMILES:	CC(C)CCCOC(=O)COCC(=O)Oc1c(Cl)cccc1Cl
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	2944.00		NIST Webbook
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tb	851.54	K	Joback Method
tc	1064.03	K	Joback Method
tf	532.93	K	Joback Method
vc	0.982	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0002456	Paxs	586.03	Joback Method
dvisc	0.0001608	Paxs	639.13	Joback Method
dvisc	0.0001123	Paxs	692.24	Joback Method
dvisc	0.0000826	Paxs	745.34	Joback Method
dvisc	0.0000633	Paxs	798.44	Joback Method
dvisc	0.0000501	Paxs	851.54	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=U382300&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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