

Diglycolic acid, 2-chlorophenyl isohexyl ester

Inchi:	InChI=1S/C16H21ClO5/c1-12(2)6-5-9-21-15(18)10-20-11-16(19)22-14-8-4-3-7-13(14)17
InchiKey:	HNAUSFBDTVHHSF-UHFFFAOYSA-N
Formula:	C16H21ClO5
SMILES:	CC(C)CCCOC(=O)COCC(=O)Oc1ccccc1Cl
Mol. weight [g/mol]:	328.79

Physical Properties

Property code	Value	Unit	Source
gf	-400.59	kJ/mol	Joback Method
hf	-791.35	kJ/mol	Joback Method
hfus	38.28	kJ/mol	Joback Method
hvap	78.87	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	3.241		Crippen Method
mcvol	245.530	ml/mol	McGowan Method
pc	1747.74	kPa	Joback Method
rinpola	2790.00		NIST Webbook
rinpola	2790.00		NIST Webbook
tb	809.13	K	Joback Method
tc	1016.81	K	Joback Method
tf	490.49	K	Joback Method
vc	0.932	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	703.05	J/molxK	809.13	Joback Method
cpg	761.11	J/molxK	982.20	Joback Method
cpg	751.65	J/molxK	947.58	Joback Method
cpg	741.11	J/molxK	912.97	Joback Method
cpg	729.50	J/molxK	878.36	Joback Method
cpg	716.81	J/molxK	843.74	Joback Method
cpg	769.51	J/molxK	1016.81	Joback Method
dvisc	0.0000574	Paxs	809.13	Joback Method

dvisc	0.0000736	Paxs	756.02	Joback Method
dvisc	0.0000981	Paxs	702.92	Joback Method
dvisc	0.0001369	Paxs	649.81	Joback Method
dvisc	0.0002027	Paxs	596.70	Joback Method
dvisc	0.0003241	Paxs	543.60	Joback Method
dvisc	0.0005736	Paxs	490.49	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=U381973&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

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