Diglycolic acid, 4-chloro-2-methylphenyl isohexyl ester

Inchi: InChI=1S/C17H23ClO5/c1-12(2)5-4-8-22-16(19)10-21-11-17(20)23-15-7-6-14(18)9-13(15

InchiKey: YFUGMMPEEARKTC-UHFFFAOYSA-N

Formula: C17H23ClO5

SMILES: Cc1cc(Cl)ccc1OC(=O)COCC(=O)OCCCC(C)C

Mol. weight [g/mol]: 342.81

Physical Properties

Property code	Value	Unit	Source
gf	-401.80	kJ/mol	Joback Method
hf	-823.46	kJ/mol	Joback Method
hfus	40.48	kJ/mol	Joback Method
hvap	81.75	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	3.550		Crippen Method
mcvol	259.620	ml/mol	McGowan Method
pc	1596.17	kPa	Joback Method
rinpol	2906.00		NIST Webbook
rinpol	2906.00		NIST Webbook
tb	836.99	K	Joback Method
tc	1044.66	K	Joback Method
tf	514.28	K	Joback Method
vc	0.989	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	758.57	J/mol×K	836.99	Joback Method
cpg	772.45	J/mol×K	871.60	Joback Method
cpg	785.21	J/mol×K	906.21	Joback Method
cpg	796.85	J/mol×K	940.83	Joback Method
cpg	807.35	J/mol×K	975.44	Joback Method
cpg	816.72	J/mol×K	1010.05	Joback Method
cpg	824.96	J/mol×K	1044.66	Joback Method
dvisc	0.0004467	Pa×s	514.28	Joback Method

dvisc	0.0002614	Pa×s	568.06	Joback Method
dvisc	0.0001678	Pa×s	621.85	Joback Method
dvisc	0.0001156	Pa×s	675.63	Joback Method
dvisc	0.0000842	Pa×s	729.42	Joback Method
dvisc	0.0000640	Pa×s	783.20	Joback Method
dvisc	0.0000504	Pa×s	836.99	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382742&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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