Diglycolic acid, di(3-chlorophenyl) ester

Inchi: InChI=1S/C16H12Cl2O5/c17-11-3-1-5-13(7-11)22-15(19)9-21-10-16(20)23-14-6-2-4-12(1
InchiKey: WGOWEQCVOGSXNN-UHFFFAOYSA-N
Formula: C16H12Cl2O5
SMILES: O=C(COCC(=O)Oc1cccc(Cl)c1)Oc1cccc(Cl)c1
Mol. weight [g/mol]: 355.17

Physical Properties

Property code	Value	Unit	Source
gf	-307.30	kJ/mol	Joback Method
hf	-576.75	kJ/mol	Joback Method
hfus	39.66	kJ/mol	Joback Method
hvap	86.58	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	3.521		Crippen Method
mcvol	234.010	ml/mol	McGowan Method
pc	2222.89	kPa	Joback Method
rinpol	3261.00		NIST Webbook
rinpol	3261.00		NIST Webbook
tb	878.66	K	Joback Method
tc	1117.38	K	Joback Method
tf	574.35	K	Joback Method
vc	0.879	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	624.97	J/mol×K	878.66	Joback Method
cpg	662.70	J/mol×K	1077.59	Joback Method
cpg	657.67	J/mol×K	1037.81	Joback Method
cpg	651.39	J/mol×K	998.02	Joback Method
cpg	643.85	J/mol×K	958.23	Joback Method
cpg	635.04	J/mol×K	918.45	Joback Method
cpg	666.48	J/mol×K	1117.38	Joback Method
dvisc	0.0000562	Pa×s	878.66	Joback Method

dvisc	0.0000692	Pa×s	827.94	Joback Method
dvisc	0.0000875	Pa×s	777.22	Joback Method
dvisc	0.0001144	Pa×s	726.50	Joback Method
dvisc	0.0001557	Pa×s	675.79	Joback Method
dvisc	0.0002227	Pa×s	625.07	Joback Method
dvisc	0.0003394	Pa×s	574.35	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=U381774&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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