

Diglycolic acid, di(2-chlorophenyl) ester

Inchi:	InChI=1S/C16H12Cl2O5/c17-11-5-1-3-7-13(11)22-15(19)9-21-10-16(20)23-14-8-4-2-6-12
InchiKey:	ZWXFMBBJWQSPOG-UHFFFAOYSA-N
Formula:	C16H12Cl2O5
SMILES:	O=C(COCC(=O)Oc1ccccc1Cl)Oc1ccccc1Cl
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
mvol	234.010	ml/mol	McGowan Method
pc	2222.89	kPa	Joback Method
rinpol	3209.00		NIST Webbook
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tb	878.66	K	Joback Method
tc	1117.38	K	Joback Method
tf	574.35	K	Joback Method
vc	0.879	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	624.97	J/molxK	878.66	Joback Method
cpg	635.04	J/molxK	918.45	Joback Method
cpg	643.85	J/molxK	958.23	Joback Method
cpg	651.39	J/molxK	998.02	Joback Method
cpg	657.67	J/molxK	1037.81	Joback Method
cpg	662.70	J/molxK	1077.59	Joback Method
cpg	666.48	J/molxK	1117.38	Joback Method
dvisc	0.0003394	Paxs	574.35	Joback Method

dvisc	0.0002227	Paxs	625.07	Joback Method
dvisc	0.0001557	Paxs	675.79	Joback Method
dvisc	0.0001144	Paxs	726.50	Joback Method
dvisc	0.0000875	Paxs	777.22	Joback Method
dvisc	0.0000692	Paxs	827.94	Joback Method
dvisc	0.0000562	Paxs	878.66	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U381978&Units=SI

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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