

Diglycolic acid, 2-chlorophenyl isobutyl ester

Inchi:	InChI=1S/C14H17ClO5/c1-10(2)7-19-13(16)8-18-9-14(17)20-12-6-4-3-5-11(12)15/h3-6,1
InchiKey:	ILAJZHDALWXPCY-UHFFFAOYSA-N
Formula:	C14H17ClO5
SMILES:	CC(C)COC(=O)COCC(=O)Oc1ccccc1Cl
Mol. weight [g/mol]:	300.74

Physical Properties

Property code	Value	Unit	Source
gf	-417.43	kJ/mol	Joback Method
hf	-750.07	kJ/mol	Joback Method
hfus	33.10	kJ/mol	Joback Method
hvap	74.42	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	2.461		Crippen Method
mcvol	217.350	ml/mol	McGowan Method
pc	2066.12	kPa	Joback Method
rinpola	2522.00		NIST Webbook
rinpola	2522.00		NIST Webbook
tb	763.37	K	Joback Method
tc	974.49	K	Joback Method
tf	467.95	K	Joback Method
vc	0.821	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	592.80	J/molxK	763.37	Joback Method
cpg	605.99	J/molxK	798.56	Joback Method
cpg	618.19	J/molxK	833.74	Joback Method
cpg	629.41	J/molxK	868.93	Joback Method
cpg	639.63	J/molxK	904.12	Joback Method
cpg	648.84	J/molxK	939.30	Joback Method
cpg	657.06	J/molxK	974.49	Joback Method
dvisc	0.0006922	Paxs	467.95	Joback Method

dvisc	0.0004014	Paxs	517.19	Joback Method
dvisc	0.0002559	Paxs	566.42	Joback Method
dvisc	0.0001753	Paxs	615.66	Joback Method
dvisc	0.0001270	Paxs	664.90	Joback Method
dvisc	0.0000962	Paxs	714.13	Joback Method
dvisc	0.0000755	Paxs	763.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381970&Units=SI
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

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
mccvol:	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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