Diglycolic acid, 4-chlorophenyl isobutyl ester

Inchi: InChI=1S/C14H17ClO5/c1-10(2)7-19-13(16)8-18-9-14(17)20-12-5-3-11(15)4-6-12/h3-6,1
InchiKey: XQYILQLTZDKKCY-UHFFFAOYSA-N
Formula: C14H17ClO5
SMILES: CC(C)COC(=O)COCC(=O)Oc1ccc(Cl)cc1
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
rinpol	2560.00		NIST Webbook
rinpol	2560.00		NIST Webbook
tb	763.37	K	Joback Method
tc	974.49	K	Joback Method
tf	467.95	K	Joback Method
vc	0.821	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0004014	Pa×s	517.19	Joback Method
dvisc	0.0002559	Pa×s	566.42	Joback Method
dvisc	0.0001753	Pa×s	615.66	Joback Method
dvisc	0.0001270	Pa×s	664.90	Joback Method
dvisc	0.0000962	Pa×s	714.13	Joback Method
dvisc	0.0000755	Pa×s	763.37	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=U381777&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