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

Inchi: InChI=1S/C13H15ClO5/c1-3-18-12(15)7-17-8-13(16)19-11-5-4-10(14)6-9(11)2/h4-6H,3,7

InchiKey: CUJICHCDEOBLGE-UHFFFAOYSA-N

Formula: C13H15ClO5

SMILES: CCOC(=O)COCC(=O)Oc1ccc(Cl)cc1C

Mol. weight [g/mol]: 286.71

Physical Properties

Property code	Value	Unit	Source
gf	-433.04	kJ/mol	Joback Method
hf	-735.62	kJ/mol	Joback Method
hfus	33.65	kJ/mol	Joback Method
hvap	73.24	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	2.134		Crippen Method
mcvol	203.260	ml/mol	McGowan Method
pc	2210.37	kPa	Joback Method
rinpol	2458.00		NIST Webbook
rinpol	2458.00		NIST Webbook
tb	745.91	K	Joback Method
tc	956.93	K	Joback Method
tf	484.20	K	Joback Method
vc	0.770	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.41	J/mol×K	745.91	Joback Method
cpg	549.91	J/mol×K	781.08	Joback Method
cpg	561.51	J/mol×K	816.25	Joback Method
cpg	572.22	J/mol×K	851.42	Joback Method
cpg	582.02	J/mol×K	886.59	Joback Method
cpg	590.88	J/mol×K	921.76	Joback Method
cpg	598.81	J/mol×K	956.93	Joback Method
dvisc	0.0005717	Pa×s	484.20	Joback Method

dvisc	0.0003734	Pa×s	527.82	Joback Method
dvisc	0.0002603	Pa×s	571.44	Joback Method
dvisc	0.0001910	Pa×s	615.06	Joback Method
dvisc	0.0001460	Pa×s	658.67	Joback Method
dvisc	0.0001154	Pa×s	702.29	Joback Method
dvisc	0.0000937	Pa×s	745.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382738&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

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