Diglycolic acid, 3-chlorophenyl ethyl ester

Inchi: InChI=1S/C12H13ClO5/c1-2-17-11(14)7-16-8-12(15)18-10-5-3-4-9(13)6-10/h3-6H,2,7-8H
InchiKey: SGBAQKDNTLOOIG-UHFFFAOYSA-N
Formula: C12H13ClO5
SMILES: CCOC(=O)COCC(=O)Oc1cccc(Cl)c1
Mol. weight [g/mol]: 272.68

Physical Properties

Property code	Value	Unit	Source
gf	-431.83	kJ/mol	Joback Method
hf	-703.51	kJ/mol	Joback Method
hfus	31.45	kJ/mol	Joback Method
hvap	70.35	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	1.825		Crippen Method
mcvol	189.170	ml/mol	McGowan Method
pc	2460.47	kPa	Joback Method
rinpol	2357.00		NIST Webbook
rinpol	2357.00		NIST Webbook
tb	718.05	K	Joback Method
tc	931.00	K	Joback Method
tf	460.41	K	Joback Method
vc	0.715	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	486.30	J/mol×K	718.05	Joback Method
cpg	538.35	J/mol×K	895.51	Joback Method
cpg	529.68	J/mol×K	860.02	Joback Method
cpg	520.13	J/mol×K	824.53	Joback Method
cpg	509.71	J/mol×K	789.03	Joback Method
cpg	498.43	J/mol×K	753.54	Joback Method
cpg	546.13	J/mol×K	931.00	Joback Method
dvisc	0.0001062	Pa×s	718.05	Joback Method

dvisc	0.0001320	Pa×s	675.11	Joback Method
dvisc	0.0001689	Pa×s	632.17	Joback Method
dvisc	0.0002241	Pa×s	589.23	Joback Method
dvisc	0.0003108	Pa×s	546.29	Joback Method
dvisc	0.0004558	Pa×s	503.35	Joback Method
dvisc	0.0007181	Pa×s	460.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381765&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