Diglycolic acid, 2,6-dichlorophenyl isobutyl ester

Inchi: InChI=1S/C14H16Cl2O5/c1-9(2)6-20-12(17)7-19-8-13(18)21-14-10(15)4-3-5-11(14)16/h3

InchiKey: NYIZQQIMJPZHTB-UHFFFAOYSA-N

Formula: C14H16Cl2O5

SMILES: CC(C)COC(=O)COCC(=O)Oc1c(Cl)cccc1Cl

Mol. weight [g/mol]: 335.18

Physical Properties

Property code	Value	Unit	Source
gf	-438.99	kJ/mol	Joback Method
hf	-777.28	kJ/mol	Joback Method
hfus	36.91	kJ/mol	Joback Method
hvap	79.46	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	3.115		Crippen Method
mcvol	229.590	ml/mol	McGowan Method
pc	1971.80	kPa	Joback Method
rinpol	2669.00		NIST Webbook
rinpol	2669.00		NIST Webbook
tb	805.78	K	Joback Method
tc	1021.07	K	Joback Method
tf	510.39	K	Joback Method
vc	0.870	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	615.26	J/mol×K	805.78	Joback Method
cpg	627.20	J/mol×K	841.66	Joback Method
cpg	638.12	J/mol×K	877.54	Joback Method
cpg	648.01	J/mol×K	913.43	Joback Method
cpg	656.87	J/mol×K	949.31	Joback Method
cpg	664.69	J/mol×K	985.19	Joback Method
cpg	671.46	J/mol×K	1021.07	Joback Method
dvisc	0.0004965	Pa×s	510.39	Joback Method

dvisc	0.0003065	Pa×s	559.62	Joback Method
dvisc	0.0002046	Pa×s	608.85	Joback Method
dvisc	0.0001450	Pa×s	658.09	Joback Method
dvisc	0.0001079	Pa×s	707.32	Joback Method
dvisc	0.0000834	Pa×s	756.55	Joback Method
dvisc	0.0000665	Pa×s	805.78	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382297&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