Diglycolic acid, isobutyl 2,4,6-trichlorophenyl ester

Inchi: InChI=1S/C14H15Cl3O5/c1-8(2)5-21-12(18)6-20-7-13(19)22-14-10(16)3-9(15)4-11(14)17

InchiKey: NVYHZCGKBVPWNX-UHFFFAOYSA-N

Formula: C14H15Cl3O5

SMILES: CC(C)COC(=O)COCC(=O)Oc1c(Cl)cc(Cl)cc1Cl

Mol. weight [g/mol]: 369.62

Physical Properties

Property code	Value	Unit	Source
gf	-460.55	kJ/mol	Joback Method
hf	-804.49	kJ/mol	Joback Method
hfus	40.72	kJ/mol	Joback Method
hvap	84.51	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.768		Crippen Method
mcvol	241.830	ml/mol	McGowan Method
pc	1883.80	kPa	Joback Method
rinpol	2812.00		NIST Webbook
rinpol	2812.00		NIST Webbook
tb	848.19	K	Joback Method
tc	1067.72	K	Joback Method
tf	552.83	K	Joback Method
vc	0.918	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	635.60	J/mol×K	848.19	Joback Method
cpg	646.25	J/mol×K	884.78	Joback Method
cpg	655.85	J/mol×K	921.37	Joback Method
cpg	664.38	J/mol×K	957.95	Joback Method
cpg	671.83	J/mol×K	994.54	Joback Method
cpg	678.17	J/mol×K	1031.13	Joback Method
cpg	683.40	J/mol×K	1067.72	Joback Method
dvisc	0.0003656	Pa×s	552.83	Joback Method

dvisc	0.0002375	Pa×s	602.06	Joback Method
dvisc	0.0001646	Pa×s	651.28	Joback Method
dvisc	0.0001201	Pa×s	700.51	Joback Method
dvisc	0.0000914	Pa×s	749.74	Joback Method
dvisc	0.0000719	Pa×s	798.96	Joback Method
dvisc	0.0000582	Pa×s	848.19	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382733&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