Diglycolic acid, 2-chloro-6-fluorophenyl isobutyl ester

Inchi: InChI=1S/C14H16ClFO5/c1-9(2)6-20-12(17)7-19-8-13(18)21-14-10(15)4-3-5-11(14)16/h3

InchiKey: PGSUEGREMXMQLZ-UHFFFAOYSA-N

Formula: C14H16ClFO5

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

Mol. weight [g/mol]: 318.73

Physical Properties

Property code	Value	Unit	Source
gf	-621.87	kJ/mol	Joback Method
hf	-957.65	kJ/mol	Joback Method
hfus	35.79	kJ/mol	Joback Method
hvap	74.26	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	2.600		Crippen Method
mcvol	219.120	ml/mol	McGowan Method
pc	1957.87	kPa	Joback Method
rinpol	2456.00		NIST Webbook
rinpol	2456.00		NIST Webbook
tb	767.62	K	Joback Method
tc	972.47	K	Joback Method
tf	481.06	K	Joback Method
vc	0.839	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.32	J/mol×K	767.62	Joback Method
cpg	611.89	J/mol×K	801.76	Joback Method
cpg	623.54	J/mol×K	835.90	Joback Method
cpg	634.26	J/mol×K	870.05	Joback Method
cpg	644.04	J/mol×K	904.19	Joback Method
cpg	652.88	J/mol×K	938.33	Joback Method
cpg	660.76	J/mol×K	972.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381940&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
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