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

Inchi: InChI=1S/C14H16ClFO5/c1-2-3-7-20-12(17)8-19-9-13(18)21-14-10(15)5-4-6-11(14)16/h4

InchiKey: HTCABCYLRYHDNW-UHFFFAOYSA-N

Formula: C14H16ClFO5

SMILES: CCCCOC(=O)COCC(=O)Oc1c(F)cccc1Cl

Mol. weight [g/mol]: 318.73

Physical Properties

Property code	Value	Unit	Source
gf	-619.43	kJ/mol	Joback Method
hf	-952.37	kJ/mol	Joback Method
hfus	39.32	kJ/mol	Joback Method
hvap	74.65	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	2.744		Crippen Method
mcvol	219.120	ml/mol	McGowan Method
pc	1944.08	kPa	Joback Method
rinpol	2511.00		NIST Webbook
rinpol	2511.00		NIST Webbook
tb	768.06	K	Joback Method
tc	970.12	K	Joback Method
tf	496.06	K	Joback Method
vc	0.845	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.74	J/mol×K	768.06	Joback Method
cpg	611.13	J/mol×K	801.74	Joback Method
cpg	622.64	J/mol×K	835.41	Joback Method
cpg	633.25	J/mol×K	869.09	Joback Method
cpg	642.97	J/mol×K	902.77	Joback Method
cpg	651.77	J/mol×K	936.44	Joback Method
cpg	659.65	J/mol×K	970.12	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=U381941&Units=SI

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