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

Inchi: InChI=1S/C16H20ClFO5/c1-2-3-4-5-9-22-14(19)10-21-11-15(20)23-16-12(17)7-6-8-13(1

InchiKey: ULSPKRIOJJHPPT-UHFFFAOYSA-N

Formula: C16H20ClFO5

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

Mol. weight [g/mol]: 346.78

Physical Properties

Property code	Value	Unit	Source
gf	-602.59	kJ/mol	Joback Method
hf	-993.65	kJ/mol	Joback Method
hfus	44.50	kJ/mol	Joback Method
hvap	79.10	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	3.525		Crippen Method
mcvol	247.300	ml/mol	McGowan Method
pc	1652.46	kPa	Joback Method
rinpol	2897.00		NIST Webbook
rinpol	2897.00		NIST Webbook
tb	813.82	K	Joback Method
tc	1014.41	K	Joback Method
tf	518.60	K	Joback Method
vc	0.957	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	708.94	J/mol×K	813.82	Joback Method
cpg	722.01	J/mol×K	847.25	Joback Method
cpg	734.08	J/mol×K	880.68	Joback Method
cpg	745.16	J/mol×K	914.11	Joback Method
cpg	755.25	J/mol×K	947.54	Joback Method
cpg	764.33	J/mol×K	980.98	Joback Method
cpg	772.42	J/mol×K	1014.41	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=U381944&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