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

Inchi: InChI=1S/C12H12ClFO5/c1-2-18-10(15)6-17-7-11(16)19-12-8(13)4-3-5-9(12)14/h3-5H,2

InchiKey: LENPPBDOXUEACY-UHFFFAOYSA-N

Formula: C12H12ClFO5

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

Mol. weight [g/mol]: 290.67

Physical Properties

Property code	Value	Unit	Source
gf	-636.27	kJ/mol	Joback Method
hf	-911.09	kJ/mol	Joback Method
hfus	34.14	kJ/mol	Joback Method
hvap	70.20	kJ/mol	Joback Method
log10ws	-2.43		Crippen Method
logp	1.964		Crippen Method
mcvol	190.940	ml/mol	McGowan Method
pc	2320.31	kPa	Joback Method
rinpol	2254.00		NIST Webbook
tb	722.30	K	Joback Method
tc	928.03	K	Joback Method
tf	473.52	K	Joback Method
vc	0.733	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.88	J/mol×K	722.30	Joback Method
cpg	504.36	J/mol×K	756.59	Joback Method
cpg	515.06	J/mol×K	790.88	Joback Method
cpg	524.98	J/mol×K	825.17	Joback Method
cpg	534.09	J/mol×K	859.46	Joback Method
cpg	542.37	J/mol×K	893.75	Joback Method
cpg	549.83	J/mol×K	928.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381938&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

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