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

Inchi: InChI=1S/C18H24ClFO5/c1-2-3-4-5-6-7-11-24-16(21)12-23-13-17(22)25-18-14(19)9-8-10

InchiKey: KTLXNWRRUPNYCP-UHFFFAOYSA-N

Formula: C18H24ClFO5

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

Mol. weight [g/mol]: 374.83

Physical Properties

Property code	Value	Unit	Source
gf	-585.75	kJ/mol	Joback Method
hf	-1034.93	kJ/mol	Joback Method
hfus	49.68	kJ/mol	Joback Method
hvap	83.55	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.305		Crippen Method
mcvol	275.480	ml/mol	McGowan Method
pc	1421.85	kPa	Joback Method
rinpol	3152.00		NIST Webbook
rinpol	3152.00		NIST Webbook
tb	859.58	K	Joback Method
tc	1061.27	K	Joback Method
tf	541.14	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	822.80	J/mol×K	859.58	Joback Method
cpg	836.39	J/mol×K	893.20	Joback Method
cpg	848.88	J/mol×K	926.81	Joback Method
cpg	860.26	J/mol×K	960.43	Joback Method
cpg	870.53	J/mol×K	994.04	Joback Method
cpg	879.71	J/mol×K	1027.66	Joback Method
cpg	887.79	J/mol×K	1061.27	Joback Method

Sources

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=U381946&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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