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

Inchi: InChI=1S/C15H18ClFO5/c1-2-3-4-8-21-13(18)9-20-10-14(19)22-15-11(16)6-5-7-12(15)1

InchiKey: OUKYKPFRLAVFGX-UHFFFAOYSA-N

Formula: C15H18ClFO5

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

Mol. weight [g/mol]: 332.75

Physical Properties

Property code	Value	Unit	Source
gf	-611.01	kJ/mol	Joback Method
hf	-973.01	kJ/mol	Joback Method
hfus	41.91	kJ/mol	Joback Method
hvap	76.87	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	3.135		Crippen Method
mcvol	233.210	ml/mol	McGowan Method
pc	1789.39	kPa	Joback Method
rinpol	2639.00		NIST Webbook
rinpol	2639.00		NIST Webbook
tb	790.94	K	Joback Method
tc	991.97	K	Joback Method
tf	507.33	K	Joback Method
vc	0.900	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.34	J/mol×K	790.94	Joback Method
cpg	666.09	J/mol×K	824.44	Joback Method
cpg	677.91	J/mol×K	857.95	Joback Method
cpg	688.78	J/mol×K	891.45	Joback Method
cpg	698.71	J/mol×K	924.96	Joback Method
cpg	707.68	J/mol×K	958.46	Joback Method
cpg	715.69	J/mol×K	991.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381942&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

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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