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

Inchi: InChI=1S/C17H22ClFO5/c1-2-3-4-5-6-10-23-15(20)11-22-12-16(21)24-17-13(18)8-7-9-14

InchiKey: BTKGWTKIYQYAQP-UHFFFAOYSA-N

Formula: C17H22ClFO5

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

Mol. weight [g/mol]: 360.81

Physical Properties

Property code	Value	Unit	Source
gf	-594.17	kJ/mol	Joback Method
hf	-1014.29	kJ/mol	Joback Method
hfus	47.09	kJ/mol	Joback Method
hvap	81.33	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	3.915		Crippen Method
mcvol	261.390	ml/mol	McGowan Method
pc	1530.66	kPa	Joback Method
rinpol	3025.00		NIST Webbook
rinpol	3025.00		NIST Webbook
tb	836.70	K	Joback Method
tc	1037.49	K	Joback Method
tf	529.87	K	Joback Method
vc	1.012	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	765.45	J/mol×K	836.70	Joback Method
cpg	778.80	J/mol×K	870.17	Joback Method
cpg	791.09	J/mol×K	903.63	Joback Method
cpg	802.34	J/mol×K	937.10	Joback Method
cpg	812.54	J/mol×K	970.56	Joback Method
cpg	821.69	J/mol×K	1004.03	Joback Method
cpg	829.80	J/mol×K	1037.49	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=U381945&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