Diglycolic acid, di(2-chloro-6-fluorophenyl) ester

Inchi: InChI=1S/C16H10Cl2F2O5/c17-9-3-1-5-11(19)15(9)24-13(21)7-23-8-14(22)25-16-10(18)4-2-6-12(16)20

InchiKey: NQZBCBAJCFLKCS-UHFFFAOYSA-N

Formula: C16H10Cl2F2O5

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

Mol. weight [g/mol]: 391.15

Physical Properties

Property code	Value	Unit	Source
gf	-716.18	kJ/mol	Joback Method
hf	-991.91	kJ/mol	Joback Method
hfus	45.04	kJ/mol	Joback Method
hvap	86.27	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	3.799		Crippen Method
mcvol	237.550	ml/mol	McGowan Method
pc	1991.21	kPa	Joback Method
rinpol	3062.00		NIST Webbook
rinpol	3062.00		NIST Webbook
tb	887.16	K	Joback Method
tc	1112.88	K	Joback Method
tf	600.57	K	Joback Method
vc	0.915	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	636.13	J/mol×K	887.16	Joback Method
cpg	645.17	J/mol×K	924.78	Joback Method
cpg	653.06	J/mol×K	962.40	Joback Method
cpg	659.79	J/mol×K	1000.02	Joback Method
cpg	665.36	J/mol×K	1037.64	Joback Method
cpg	669.75	J/mol×K	1075.26	Joback Method
cpg	672.96	J/mol×K	1112.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381950&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