Diethylmalonic acid, monochloride, 3-fluorophenyl ester

Inchi: InChI=1S/C13H14ClFO3/c1-3-13(4-2,11(14)16)12(17)18-10-7-5-6-9(15)8-10/h5-8H,3-4H

InchiKey: UKULKPHRFJVYND-UHFFFAOYSA-N

Formula: C13H14ClFO3

SMILES: CCC(CC)(C(=O)Cl)C(=O)Oc1cccc(F)c1

Mol. weight [g/mol]: 272.70

Physical Properties

Property code	Value	Unit	Source
gf	-405.38	kJ/mol	Joback Method
hf	-664.57	kJ/mol	Joback Method
hfus	27.33	kJ/mol	Joback Method
hvap	65.64	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.303		Crippen Method
mcvol	193.290	ml/mol	McGowan Method
pc	2258.96	kPa	Joback Method
rinpol	1624.00		NIST Webbook
rinpol	1624.00		NIST Webbook
tb	692.13	K	Joback Method
tc	908.25	K	Joback Method
tf	430.23	K	Joback Method
vc	0.742	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.53	J/mol×K	692.13	Joback Method
cpg	511.46	J/mol×K	728.15	Joback Method
cpg	523.45	J/mol×K	764.17	Joback Method
cpg	534.55	J/mol×K	800.19	Joback Method
cpg	544.79	J/mol×K	836.21	Joback Method
cpg	554.21	J/mol×K	872.23	Joback Method
cpg	562.88	J/mol×K	908.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370206&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