Diethylmalonic acid, monochloride, 2-chloro-6-fluorophenyl ester

Inchi: InChI=1S/C13H13Cl2FO3/c1-3-13(4-2,11(15)17)12(18)19-10-8(14)6-5-7-9(10)16/h5-7H,3

InchiKey: VFEWYRDECGUHDX-UHFFFAOYSA-N

Formula: C13H13Cl2FO3

SMILES: CCC(CC)(C(=O)Cl)C(=O)Oc1c(F)cccc1Cl

Mol. weight [g/mol]: 307.14

Physical Properties

Property code	Value	Unit	Source
gf	-426.94	kJ/mol	Joback Method
hf	-691.78	kJ/mol	Joback Method
hfus	31.14	kJ/mol	Joback Method
hvap	70.69	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	3.956		Crippen Method
mcvol	205.530	ml/mol	McGowan Method
pc	2151.31	kPa	Joback Method
rinpol	1825.00		NIST Webbook
rinpol	1825.00		NIST Webbook
tb	734.54	K	Joback Method
tc	954.51	K	Joback Method
tf	472.67	K	Joback Method
vc	0.790	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.00	J/mol×K	734.54	Joback Method
cpg	532.68	J/mol×K	771.20	Joback Method
cpg	543.47	J/mol×K	807.86	Joback Method
cpg	553.40	J/mol×K	844.53	Joback Method
cpg	562.53	J/mol×K	881.19	Joback Method
cpg	570.88	J/mol×K	917.85	Joback Method
cpg	578.51	J/mol×K	954.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369688&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