Dimethylmalonic acid, 2-chloro-6-fluorophenyl ethyl ester

Inchi: InChI=1S/C13H14ClFO4/c1-4-18-11(16)13(2,3)12(17)19-10-8(14)6-5-7-9(10)15/h5-7H,4

InchiKey: BCAPCYWCGIFVJK-UHFFFAOYSA-N

Formula: C13H14ClFO4

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

Mol. weight [g/mol]: 288.70

Physical Properties

Property code	Value	Unit	Source
gf	-520.01	kJ/mol	Joback Method
hf	-808.26	kJ/mol	Joback Method
hfus	28.13	kJ/mol	Joback Method
hvap	68.72	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	2.974		Crippen Method
mcvol	199.160	ml/mol	McGowan Method
pc	2191.78	kPa	Joback Method
rinpol	1691.00		NIST Webbook
rinpol	1691.00		NIST Webbook
tb	719.53	K	Joback Method
tc	934.22	K	Joback Method
tf	464.98	K	Joback Method
vc	0.759	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.47	J/mol×K	719.53	Joback Method
cpg	534.95	J/mol×K	755.31	Joback Method
cpg	546.54	J/mol×K	791.09	Joback Method
cpg	557.24	J/mol×K	826.87	Joback Method
cpg	567.08	J/mol×K	862.66	Joback Method
cpg	576.08	J/mol×K	898.44	Joback Method
cpg	584.27	J/mol×K	934.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361951&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