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

Inchi: InChI=1S/C14H16ClFO4/c1-4-8-19-12(17)14(2,3)13(18)20-11-9(15)6-5-7-10(11)16/h5-7H

InchiKey: GZMKLAYYFNJJGI-UHFFFAOYSA-N

Formula: C14H16ClFO4

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

Mol. weight [g/mol]: 302.73

Physical Properties

Property code	Value	Unit	Source
gf	-511.59	kJ/mol	Joback Method
hf	-828.90	kJ/mol	Joback Method
hfus	30.72	kJ/mol	Joback Method
hvap	70.94	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	3.364		Crippen Method
mcvol	213.250	ml/mol	McGowan Method
pc	2007.30	kPa	Joback Method
rinpol	1785.00		NIST Webbook
tb	742.41	K	Joback Method
tc	954.26	K	Joback Method
tf	476.25	K	Joback Method
vc	0.816	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.06	J/mol×K	742.41	Joback Method
cpg	587.98	J/mol×K	777.72	Joback Method
cpg	599.97	J/mol×K	813.03	Joback Method
cpg	611.04	J/mol×K	848.33	Joback Method
cpg	621.23	J/mol×K	883.64	Joback Method
cpg	630.56	J/mol×K	918.95	Joback Method
cpg	639.05	J/mol×K	954.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361952&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