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

Inchi: InChI=1S/C15H18ClFO4/c1-9(2)8-20-13(18)15(3,4)14(19)21-12-10(16)6-5-7-11(12)17/h5

InchiKey: PFZBZSSTOKJGPF-UHFFFAOYSA-N

Formula: C15H18ClFO4

SMILES: CC(C)COC(=O)C(C)(C)C(=O)Oc1c(F)cccc1Cl

Mol. weight [g/mol]: 316.75

Physical Properties

Property code	Value	Unit	Source
gf	-505.61	kJ/mol	Joback Method
hf	-854.82	kJ/mol	Joback Method
hfus	29.78	kJ/mol	Joback Method
hvap	72.78	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.610		Crippen Method
mcvol	227.340	ml/mol	McGowan Method
pc	1857.91	kPa	Joback Method
rinpol	1837.00		NIST Webbook
rinpol	1837.00		NIST Webbook
tb	764.85	K	Joback Method
tc	977.53	K	Joback Method
tf	472.52	K	Joback Method
vc	0.866	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	629.39	J/mol×K	764.85	Joback Method
cpg	642.88	J/mol×K	800.30	Joback Method
cpg	655.37	J/mol×K	835.74	Joback Method
cpg	666.89	J/mol×K	871.19	Joback Method
cpg	677.46	J/mol×K	906.64	Joback Method
cpg	687.11	J/mol×K	942.08	Joback Method
cpg	695.87	J/mol×K	977.53	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361953&Units=SI

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