Dimethylmalonic acid, 2-bromo-4-fluorophenyl ethyl ester

Inchi: InChI=1S/C13H14BrFO4/c1-4-18-11(16)13(2,3)12(17)19-10-6-5-8(15)7-9(10)14/h5-7H,4

InchiKey: BTIHOIGJBJUHMU-UHFFFAOYSA-N

Formula: C13H14BrFO4

SMILES: CCOC(=O)C(C)(C)C(=O)Oc1ccc(F)cc1Br

Mol. weight [g/mol]: 333.15

Physical Properties

Property code	Value	Unit	Source
gf	-493.76	kJ/mol	Joback Method
hf	-766.19	kJ/mol	Joback Method
hfus	29.21	kJ/mol	Joback Method
hvap	70.77	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.083		Crippen Method
mcvol	204.420	ml/mol	McGowan Method
pc	2426.65	kPa	Joback Method
rinpol	1735.00		NIST Webbook
rinpol	1735.00		NIST Webbook
tb	748.26	K	Joback Method
tc	970.01	K	Joback Method
tf	494.86	K	Joback Method
vc	0.772	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	533.32	J/mol×K	748.26	Joback Method
cpg	545.36	J/mol×K	785.22	Joback Method
cpg	556.48	J/mol×K	822.18	Joback Method
cpg	566.70	J/mol×K	859.13	Joback Method
cpg	576.07	J/mol×K	896.09	Joback Method
cpg	584.60	J/mol×K	933.05	Joback Method
cpg	592.34	J/mol×K	970.01	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=U361818&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