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

Inchi: InChI=1S/C14H16BrFO4/c1-4-7-19-12(17)14(2,3)13(18)20-11-6-5-9(16)8-10(11)15/h5-6,

InchiKey: WCEYACRHXILLMS-UHFFFAOYSA-N

Formula: C14H16BrFO4

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

Mol. weight [g/mol]: 347.18

Physical Properties

Property code	Value	Unit	Source
gf	-485.34	kJ/mol	Joback Method
hf	-786.83	kJ/mol	Joback Method
hfus	31.80	kJ/mol	Joback Method
hvap	72.99	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	3.473		Crippen Method
mcvol	218.510	ml/mol	McGowan Method
pc	2212.45	kPa	Joback Method
rinpol	1829.00		NIST Webbook
rinpol	1829.00		NIST Webbook
tb	771.14	K	Joback Method
tc	989.79	K	Joback Method
tf	506.13	K	Joback Method
vc	0.829	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	586.34	J/mol×K	771.14	Joback Method
cpg	598.80	J/mol×K	807.58	Joback Method
cpg	610.30	J/mol×K	844.02	Joback Method
cpg	620.89	J/mol×K	880.47	Joback Method
cpg	630.61	J/mol×K	916.91	Joback Method
cpg	639.47	J/mol×K	953.35	Joback Method
cpg	647.53	J/mol×K	989.79	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=U361819&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