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

Inchi: InChI=1S/C15H18BrFO4/c1-9(2)8-20-13(18)15(3,4)14(19)21-12-6-5-10(17)7-11(12)16/h5

InchiKey: GXJQNNBOVDBOTD-UHFFFAOYSA-N

Formula: C15H18BrFO4

SMILES: CC(C)COC(=O)C(C)(C)C(=O)Oc1ccc(F)cc1Br

Mol. weight [g/mol]: 361.20

Physical Properties

Property code	Value	Unit	Source
gf	-479.36	kJ/mol	Joback Method
hf	-812.75	kJ/mol	Joback Method
hfus	30.87	kJ/mol	Joback Method
hvap	74.83	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	3.719		Crippen Method
mcvol	232.600	ml/mol	McGowan Method
pc	2040.07	kPa	Joback Method
rinpol	1877.00		NIST Webbook
tb	793.58	K	Joback Method
tc	1012.91	K	Joback Method
tf	502.40	K	Joback Method
vc	0.878	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	641.04	J/mol×K	793.58	Joback Method
cpg	654.04	J/mol×K	830.14	Joback Method
cpg	666.03	J/mol×K	866.69	Joback Method
cpg	677.04	J/mol×K	903.25	Joback Method
cpg	687.12	J/mol×K	939.80	Joback Method
cpg	696.30	J/mol×K	976.36	Joback Method
cpg	704.61	J/mol×K	1012.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361820&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