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

Inchi: InChI=1S/C15H18BrFO4/c1-4-5-8-20-13(18)15(2,3)14(19)21-12-7-6-10(17)9-11(12)16/h6

InchiKey: LXXVERCJKFZDFQ-UHFFFAOYSA-N

Formula: C15H18BrFO4

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

Mol. weight [g/mol]: 361.20

Physical Properties

Property code	Value	Unit	Source
gf	-476.92	kJ/mol	Joback Method
hf	-807.47	kJ/mol	Joback Method
hfus	34.39	kJ/mol	Joback Method
hvap	75.22	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	3.863		Crippen Method
mcvol	232.600	ml/mol	McGowan Method
pc	2025.41	kPa	Joback Method
rinpol	1912.00		NIST Webbook
rinpol	1912.00		NIST Webbook
tb	794.02	K	Joback Method
tc	1010.11	K	Joback Method
tf	517.40	K	Joback Method
vc	0.884	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	640.46	J/mol×K	794.02	Joback Method
cpg	653.26	J/mol×K	830.03	Joback Method
cpg	665.10	J/mol×K	866.05	Joback Method
cpg	676.01	J/mol×K	902.06	Joback Method
cpg	686.02	J/mol×K	938.08	Joback Method
cpg	695.17	J/mol×K	974.09	Joback Method
cpg	703.49	J/mol×K	1010.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361821&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