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

Inchi: InChI=1S/C11H9BrClFO3/c1-11(2,9(13)15)10(16)17-8-4-3-6(14)5-7(8)12/h3-5H,1-2H3

InchiKey: ROUGUNDOWOMSGL-UHFFFAOYSA-N

Formula: C11H9BrClFO3

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

Mol. weight [g/mol]: 323.54

Physical Properties

Property code	Value	Unit	Source
gf	-417.53	kJ/mol	Joback Method
hf	-608.43	kJ/mol	Joback Method
hfus	27.04	kJ/mol	Joback Method
hvap	68.29	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	3.285		Crippen Method
mcvol	182.610	ml/mol	McGowan Method
pc	2896.73	kPa	Joback Method
rinpol	1663.00		NIST Webbook
rinpol	1663.00		NIST Webbook
tb	717.51	K	Joback Method
tc	952.74	K	Joback Method
tf	480.01	K	Joback Method
vc	0.692	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	428.81	J/mol×K	717.51	Joback Method
cpg	438.94	J/mol×K	756.72	Joback Method
cpg	448.21	J/mol×K	795.92	Joback Method
cpg	456.67	J/mol×K	835.13	Joback Method
cpg	464.38	J/mol×K	874.33	Joback Method
cpg	471.40	J/mol×K	913.54	Joback Method
cpg	477.76	J/mol×K	952.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361828&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

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