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

Inchi: InChI=1S/C19H26BrFO4/c1-4-5-6-7-8-9-12-24-17(22)19(2,3)18(23)25-16-11-10-14(21)13

InchiKey: HUWZDMYHBAGNBK-UHFFFAOYSA-N

Formula: C19H26BrFO4

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

Mol. weight [g/mol]: 417.31

Physical Properties

Property code	Value	Unit	Source
gf	-443.24	kJ/mol	Joback Method
hf	-890.03	kJ/mol	Joback Method
hfus	44.75	kJ/mol	Joback Method
hvap	84.12	kJ/mol	Joback Method
log10ws	-6.51		Crippen Method
logp	5.423		Crippen Method
mcvol	288.960	ml/mol	McGowan Method
pc	1472.49	kPa	Joback Method
rinpol	2299.00		NIST Webbook
rinpol	2299.00		NIST Webbook
tb	885.54	K	Joback Method
tc	1097.51	K	Joback Method
tf	562.48	K	Joback Method
vc	1.109	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	866.41	J/mol×K	885.54	Joback Method
cpg	880.29	J/mol×K	920.87	Joback Method
cpg	893.11	J/mol×K	956.20	Joback Method
cpg	904.91	J/mol×K	991.52	Joback Method
cpg	915.75	J/mol×K	1026.85	Joback Method
cpg	925.66	J/mol×K	1062.18	Joback Method
cpg	934.70	J/mol×K	1097.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361825&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