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

Inchi: InChI=1S/C17H22BrFO4/c1-11(2)6-5-9-22-15(20)17(3,4)16(21)23-14-8-7-12(19)10-13(14

InchiKey: IZYKXWIDMNVRKT-UHFFFAOYSA-N

Formula: C17H22BrFO4

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

Mol. weight [g/mol]: 389.26

Physical Properties

Property code	Value	Unit	Source
gf	-462.52	kJ/mol	Joback Method
hf	-854.03	kJ/mol	Joback Method
hfus	36.05	kJ/mol	Joback Method
hvap	79.28	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	4.499		Crippen Method
mcvol	260.780	ml/mol	McGowan Method
pc	1727.46	kPa	Joback Method
rinpol	2065.00		NIST Webbook
tb	839.34	K	Joback Method
tc	1054.66	K	Joback Method
tf	524.94	K	Joback Method
vc	0.991	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	752.23	J/mol×K	839.34	Joback Method
cpg	765.77	J/mol×K	875.23	Joback Method
cpg	778.26	J/mol×K	911.11	Joback Method
cpg	789.75	J/mol×K	947.00	Joback Method
cpg	800.26	J/mol×K	982.89	Joback Method
cpg	809.86	J/mol×K	1018.77	Joback Method
cpg	818.57	J/mol×K	1054.66	Joback Method

Sources

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=U361823&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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