Dimethylmalonic acid, 3,5-difluorophenyl isohexyl ester

Inchi: InChI=1S/C17H22F2O4/c1-11(2)6-5-7-22-15(20)17(3,4)16(21)23-14-9-12(18)8-13(19)10

InchiKey: AVWHHQIIRJTIKO-UHFFFAOYSA-N

Formula: C17H22F2O4

SMILES: CC(C)CCCOC(=O)C(C)(C)C(=O)Oc1cc(F)cc(F)c1

Mol. weight [g/mol]: 328.35

Physical Properties

Property code	Value	Unit	Source
gf	-671.65	kJ/mol	Joback Method
hf	-1076.47	kJ/mol	Joback Method
hfus	33.85	kJ/mol	Joback Method
hvap	72.03	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	3.876		Crippen Method
mcvol	245.050	ml/mol	McGowan Method
pc	1574.70	kPa	Joback Method
rinpol	1771.00		NIST Webbook
rinpol	1771.00		NIST Webbook
tb	772.45	K	Joback Method
tc	971.39	K	Joback Method
tf	465.73	K	Joback Method
vc	0.947	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	721.24	J/mol×K	772.45	Joback Method
cpg	735.94	J/mol×K	805.61	Joback Method
cpg	749.64	J/mol×K	838.76	Joback Method
cpg	762.37	J/mol×K	871.92	Joback Method
cpg	774.16	J/mol×K	905.08	Joback Method
cpg	785.04	J/mol×K	938.24	Joback Method
cpg	795.03	J/mol×K	971.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361815&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