Dimethylmalonic acid, 3,5-difluorophenyl propyl ester

Inchi: InChI=1S/C14H16F2O4/c1-4-5-19-12(17)14(2,3)13(18)20-11-7-9(15)6-10(16)8-11/h6-8H

InchiKey: FOYYUTDRAJGIMI-UHFFFAOYSA-N

Formula: C14H16F2O4

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

Mol. weight [g/mol]: 286.27

Physical Properties

Property code	Value	Unit	Source
gf	-694.47	kJ/mol	Joback Method
hf	-1009.27	kJ/mol	Joback Method
hfus	29.60	kJ/mol	Joback Method
hvap	65.74	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	2.850		Crippen Method
mcvol	202.780	ml/mol	McGowan Method
pc	1992.98	kPa	Joback Method
rinpol	1536.00		NIST Webbook
rinpol	1536.00		NIST Webbook
tb	704.25	K	Joback Method
tc	904.93	K	Joback Method
tf	446.92	K	Joback Method
vc	0.784	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	557.54	J/mol×K	704.25	Joback Method
cpg	570.97	J/mol×K	737.70	Joback Method
cpg	583.52	J/mol×K	771.14	Joback Method
cpg	595.23	J/mol×K	804.59	Joback Method
cpg	606.10	J/mol×K	838.04	Joback Method
cpg	616.17	J/mol×K	871.49	Joback Method
cpg	625.44	J/mol×K	904.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361812&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