Dimethylmalonic acid, hexadecyl 2,3,4-trifluorophenyl ester

Inchi: InChI=1S/C27H41F3O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-33-25(31)27(2,3)26

InchiKey: UAFSFRUDLVMEGS-UHFFFAOYSA-N

Formula: C27H41F3O4

SMILES: CCCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1ccc(F)c(F)c1F

Mol. weight [g/mol]: 486.61

Physical Properties

Property code	Value	Unit	Source
gf	-789.45	kJ/mol	Joback Method
hf	-1485.17	kJ/mol	Joback Method
hfus	65.96	kJ/mol	Joback Method
hvap	94.52	kJ/mol	Joback Method
log10ws	-9.35		Crippen Method
logp	8.060		Crippen Method
mcvol	387.720	ml/mol	McGowan Method
pc	794.39	kPa	Joback Method
rinpol	2823.00		NIST Webbook
rinpol	2823.00		NIST Webbook
tb	1005.94	K	Joback Method
tc	1238.26	K	Joback Method
tf	606.54	K	Joback Method
vc	1.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1325.20	J/mol×K	1005.94	Joback Method
cpg	1342.79	J/mol×K	1044.66	Joback Method
cpg	1358.76	J/mol×K	1083.38	Joback Method
cpg	1373.18	J/mol×K	1122.10	Joback Method
cpg	1386.13	J/mol×K	1160.82	Joback Method
cpg	1397.70	J/mol×K	1199.54	Joback Method
cpg	1407.94	J/mol×K	1238.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361894&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