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

Inchi: InChI=1S/C23H33F3O4/c1-4-5-6-7-8-9-10-11-12-13-16-29-21(27)23(2,3)22(28)30-18-15

InchiKey: ATIIFKVUZFIFRE-UHFFFAOYSA-N

Formula: C23H33F3O4

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

Mol. weight [g/mol]: 430.50

Physical Properties

Property code	Value	Unit	Source
gf	-823.13	kJ/mol	Joback Method
hf	-1402.61	kJ/mol	Joback Method
hfus	55.60	kJ/mol	Joback Method
hvap	85.62	kJ/mol	Joback Method
log10ws	-7.68		Crippen Method
logp	6.500		Crippen Method
mcvol	331.360	ml/mol	McGowan Method
pc	998.91	kPa	Joback Method
rinpol	2437.00		NIST Webbook
rinpol	2437.00		NIST Webbook
tb	914.42	K	Joback Method
tc	1119.62	K	Joback Method
tf	561.46	K	Joback Method
vc	1.306	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1078.44	J/mol×K	914.42	Joback Method
cpg	1094.36	J/mol×K	948.62	Joback Method
cpg	1109.06	J/mol×K	982.82	Joback Method
cpg	1122.57	J/mol×K	1017.02	Joback Method
cpg	1134.95	J/mol×K	1051.22	Joback Method
cpg	1146.23	J/mol×K	1085.42	Joback Method
cpg	1156.45	J/mol×K	1119.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361890&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