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

Inchi: InChI=1S/C21H29F3O4/c1-4-5-6-7-8-9-10-11-14-27-19(25)21(2,3)20(26)28-16-13-12-15

InchiKey: VHBIIHDIEFWJOI-UHFFFAOYSA-N

Formula: C21H29F3O4

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

Mol. weight [g/mol]: 402.45

Physical Properties

Property code	Value	Unit	Source
gf	-839.97	kJ/mol	Joback Method
hf	-1361.33	kJ/mol	Joback Method
hfus	50.42	kJ/mol	Joback Method
hvap	81.17	kJ/mol	Joback Method
log10ws	-6.84		Crippen Method
logp	5.719		Crippen Method
mcvol	303.180	ml/mol	McGowan Method
pc	1132.15	kPa	Joback Method
rinpol	2239.00		NIST Webbook
tb	868.66	K	Joback Method
tc	1066.36	K	Joback Method
tf	538.92	K	Joback Method
vc	1.194	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	958.42	J/mol×K	868.66	Joback Method
cpg	973.66	J/mol×K	901.61	Joback Method
cpg	987.82	J/mol×K	934.56	Joback Method
cpg	1000.91	J/mol×K	967.51	Joback Method
cpg	1012.97	J/mol×K	1000.46	Joback Method
cpg	1024.04	J/mol×K	1033.41	Joback Method
cpg	1034.14	J/mol×K	1066.36	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361888&Units=SI

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