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

Inchi: InChI=1S/C22H31F3O4/c1-4-5-6-7-8-9-10-11-12-15-28-20(26)22(2,3)21(27)29-17-14-13

InchiKey: JFCKUISHCGKTSH-UHFFFAOYSA-N

Formula: C22H31F3O4

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

Mol. weight [g/mol]: 416.47

Physical Properties

Property code	Value	Unit	Source
gf	-831.55	kJ/mol	Joback Method
hf	-1381.97	kJ/mol	Joback Method
hfus	53.01	kJ/mol	Joback Method
hvap	83.39	kJ/mol	Joback Method
log10ws	-7.26		Crippen Method
logp	6.109		Crippen Method
mcvol	317.270	ml/mol	McGowan Method
pc	1062.40	kPa	Joback Method
rinpol	2338.00		NIST Webbook
rinpol	2338.00		NIST Webbook
tb	891.54	K	Joback Method
tc	1092.54	K	Joback Method
tf	550.19	K	Joback Method
vc	1.250	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1018.10	J/mol×K	891.54	Joback Method
cpg	1033.68	J/mol×K	925.04	Joback Method
cpg	1048.10	J/mol×K	958.54	Joback Method
cpg	1061.40	J/mol×K	992.04	Joback Method
cpg	1073.62	J/mol×K	1025.54	Joback Method
cpg	1084.80	J/mol×K	1059.04	Joback Method
cpg	1094.97	J/mol×K	1092.54	Joback Method

Sources

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=U361889&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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