Dimethylmalonic acid, dodecyl 2-fluoro-3-trifluoromethylphenyl ester

Inchi: InChI=1S/C24H34F4O4/c1-4-5-6-7-8-9-10-11-12-13-17-31-21(29)23(2,3)22(30)32-19-16
InchiKey: CWZJBEKAXDWLHL-UHFFFAOYSA-N
Formula: C24H34F4O4
SMILES: CCCCCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1cccc(C(F)(F)F)c1F
Mol. weight [g/mol]: 462.52

Physical Properties

Property code	Value	Unit	Source
gf	-997.05	kJ/mol	Joback Method
hf	-1616.64	kJ/mol	Joback Method
hfus	54.24	kJ/mol	Joback Method
hvap	85.07	kJ/mol	Joback Method
log10ws	-8.12		Crippen Method
logp	7.240		Crippen Method
mcvol	347.220	ml/mol	McGowan Method
pc	934.63	kPa	Joback Method
rinpol	2428.00		NIST Webbook
rinpol	2428.00		NIST Webbook
tb	928.36	K	Joback Method
tc	1136.58	K	Joback Method
tf	563.22	K	Joback Method
vc	1.369	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1147.25	J/mol×K	928.36	Joback Method
cpg	1163.34	J/mol×K	963.06	Joback Method
cpg	1178.24	J/mol×K	997.77	Joback Method
cpg	1192.02	J/mol×K	1032.47	Joback Method
cpg	1204.75	J/mol×K	1067.17	Joback Method
cpg	1216.51	J/mol×K	1101.88	Joback Method
cpg	1227.37	J/mol×K	1136.58	Joback Method

Sources

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=U362004&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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