Dimethylmalonic acid, 2-chloro-6-fluorophenyl undecyl ester

Inchi: InChI=1S/C22H32ClFO4/c1-4-5-6-7-8-9-10-11-12-16-27-20(25)22(2,3)21(26)28-19-17(23
InchiKey: WCLTUOXFBNCFPM-UHFFFAOYSA-N
Formula: C22H32ClFO4
SMILES: CCCCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1c(F)cccc1Cl
Mol. weight [g/mol]: 414.94

Physical Properties

Property code	Value	Unit	Source
gf	-444.23	kJ/mol	Joback Method
hf	-994.02	kJ/mol	Joback Method
hfus	51.44	kJ/mol	Joback Method
hvap	88.75	kJ/mol	Joback Method
log10ws	-7.28		Crippen Method
logp	6.485		Crippen Method
mcvol	325.970	ml/mol	McGowan Method
pc	1111.11	kPa	Joback Method
rinpol	2570.00		NIST Webbook
tb	925.45	K	Joback Method
tc	1135.93	K	Joback Method
tf	566.41	K	Joback Method
vc	1.264	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1030.98	J/mol×K	925.45	Joback Method
cpg	1046.05	J/mol×K	960.53	Joback Method
cpg	1059.92	J/mol×K	995.61	Joback Method
cpg	1072.64	J/mol×K	1030.69	Joback Method
cpg	1084.26	J/mol×K	1065.77	Joback Method
cpg	1094.83	J/mol×K	1100.85	Joback Method
cpg	1104.39	J/mol×K	1135.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361961&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