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

Inchi: InChI=1S/C27H42ClFO4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21-32-25(30)27(2,3)26

InchiKey: YYXSVZYERYDSNU-UHFFFAOYSA-N

Formula: C27H42ClFO4

SMILES: CCCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1c(F)cccc1Cl

Mol. weight [g/mol]: 485.07

Physical Properties

Property code	Value	Unit	Source
gf	-402.13	kJ/mol	Joback Method
hf	-1097.22	kJ/mol	Joback Method
hfus	64.39	kJ/mol	Joback Method
hvap	99.88	kJ/mol	Joback Method
log10ws	-9.38		Crippen Method
logp	8.435		Crippen Method
mcvol	396.420	ml/mol	McGowan Method
pc	825.74	kPa	Joback Method
rinpol	3089.00		NIST Webbook
rinpol	3089.00		NIST Webbook
tb	1039.85	K	Joback Method
tc	1276.78	K	Joback Method
tf	622.76	K	Joback Method
vc	1.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1337.95	J/mol×K	1039.85	Joback Method
cpg	1354.55	J/mol×K	1079.34	Joback Method
cpg	1369.60	J/mol×K	1118.83	Joback Method
cpg	1383.18	J/mol×K	1158.31	Joback Method
cpg	1395.38	J/mol×K	1197.80	Joback Method
cpg	1406.30	J/mol×K	1237.29	Joback Method
cpg	1416.02	J/mol×K	1276.78	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=U361966&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