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

Inchi: InChI=1S/C23H34ClFO4/c1-4-5-6-7-8-9-10-11-12-13-17-28-21(26)23(2,3)22(27)29-20-18

InchiKey: XJPAROOCAYDPSK-UHFFFAOYSA-N

Formula: C23H34ClFO4

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

Mol. weight [g/mol]: 428.96

Physical Properties

Property code	Value	Unit	Source
gf	-435.81	kJ/mol	Joback Method
hf	-1014.66	kJ/mol	Joback Method
hfus	54.03	kJ/mol	Joback Method
hvap	90.98	kJ/mol	Joback Method
log10ws	-7.70		Crippen Method
logp	6.875		Crippen Method
mcvol	340.060	ml/mol	McGowan Method
pc	1043.27	kPa	Joback Method
rinpol	2666.00		NIST Webbook
rinpol	2666.00		NIST Webbook
tb	948.33	K	Joback Method
tc	1162.05	K	Joback Method
tf	577.68	K	Joback Method
vc	1.319	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1091.35	J/mol×K	948.33	Joback Method
cpg	1106.67	J/mol×K	983.95	Joback Method
cpg	1120.74	J/mol×K	1019.57	Joback Method
cpg	1133.61	J/mol×K	1055.19	Joback Method
cpg	1145.34	J/mol×K	1090.81	Joback Method
cpg	1155.98	J/mol×K	1126.43	Joback Method
cpg	1165.59	J/mol×K	1162.05	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=U361962&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