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

Inchi: InChI=1S/C21H30ClFO4/c1-4-5-6-7-8-9-10-11-15-26-19(24)21(2,3)20(25)27-18-16(22)13

InchiKey: GKIDJWPMOLGVNZ-UHFFFAOYSA-N

Formula: C21H30ClFO4

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

Mol. weight [g/mol]: 400.91

Physical Properties

Property code	Value	Unit	Source
gf	-452.65	kJ/mol	Joback Method
hf	-973.38	kJ/mol	Joback Method
hfus	48.85	kJ/mol	Joback Method
hvap	86.52	kJ/mol	Joback Method
log10ws	-6.86		Crippen Method
logp	6.095		Crippen Method
mcvol	311.880	ml/mol	McGowan Method
pc	1185.79	kPa	Joback Method
rinpol	2472.00		NIST Webbook
rinpol	2472.00		NIST Webbook
tb	902.57	K	Joback Method
tc	1110.69	K	Joback Method
tf	555.14	K	Joback Method
vc	1.208	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	971.22	J/mol×K	902.57	Joback Method
cpg	986.05	J/mol×K	937.26	Joback Method
cpg	999.73	J/mol×K	971.94	Joback Method
cpg	1012.30	J/mol×K	1006.63	Joback Method
cpg	1023.81	J/mol×K	1041.32	Joback Method
cpg	1034.30	J/mol×K	1076.00	Joback Method
cpg	1043.81	J/mol×K	1110.69	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=U361960&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