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

Inchi: InChI=1S/C26H40ClFO4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-20-31-24(29)26(2,3)25(30

InchiKey: WOFRFGLBJULXBX-UHFFFAOYSA-N

Formula: C26H40ClFO4

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

Mol. weight [g/mol]: 471.05

Physical Properties

Property code	Value	Unit	Source
gf	-410.55	kJ/mol	Joback Method
hf	-1076.58	kJ/mol	Joback Method
hfus	61.80	kJ/mol	Joback Method
hvap	97.65	kJ/mol	Joback Method
log10ws	-8.96		Crippen Method
logp	8.045		Crippen Method
mcvol	382.330	ml/mol	McGowan Method
pc	873.25	kPa	Joback Method
rinpol	2986.00		NIST Webbook
rinpol	2986.00		NIST Webbook
tb	1016.97	K	Joback Method
tc	1246.41	K	Joback Method
tf	611.49	K	Joback Method
vc	1.488	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1275.62	J/mol×K	1016.97	Joback Method
cpg	1291.85	J/mol×K	1055.21	Joback Method
cpg	1306.62	J/mol×K	1093.45	Joback Method
cpg	1320.00	J/mol×K	1131.69	Joback Method
cpg	1332.07	J/mol×K	1169.93	Joback Method
cpg	1342.92	J/mol×K	1208.17	Joback Method
cpg	1352.61	J/mol×K	1246.41	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=U361965&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

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