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

Inchi: InChI=1S/C25H38ClFO4/c1-4-7-8-9-10-11-12-13-14-15-19-30-23(28)25(5-2,6-3)24(29)31

InchiKey: JRATWILPMMZWSV-UHFFFAOYSA-N

Formula: C25H38ClFO4

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

Mol. weight [g/mol]: 457.02

Physical Properties

Property code	Value	Unit	Source
gf	-418.97	kJ/mol	Joback Method
hf	-1055.94	kJ/mol	Joback Method
hfus	59.21	kJ/mol	Joback Method
hvap	95.43	kJ/mol	Joback Method
log10ws	-8.54		Crippen Method
logp	7.655		Crippen Method
mcvol	368.240	ml/mol	McGowan Method
pc	924.99	kPa	Joback Method
rinpol	2873.00		NIST Webbook
rinpol	2873.00		NIST Webbook
tb	994.09	K	Joback Method
tc	1217.22	K	Joback Method
tf	600.22	K	Joback Method
vc	1.431	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1213.72	J/mol×K	994.09	Joback Method
cpg	1229.62	J/mol×K	1031.28	Joback Method
cpg	1244.13	J/mol×K	1068.47	Joback Method
cpg	1257.33	J/mol×K	1105.66	Joback Method
cpg	1269.28	J/mol×K	1142.84	Joback Method
cpg	1280.06	J/mol×K	1180.03	Joback Method
cpg	1289.73	J/mol×K	1217.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369682&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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