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

Inchi: InChI=1S/C24H36ClFO4/c1-4-7-8-9-10-11-12-13-14-18-29-22(27)24(5-2,6-3)23(28)30-21

InchiKey: OSEGFJLXYHDSQM-UHFFFAOYSA-N

Formula: C24H36ClFO4

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

Mol. weight [g/mol]: 442.99

Physical Properties

Property code	Value	Unit	Source
gf	-427.39	kJ/mol	Joback Method
hf	-1035.30	kJ/mol	Joback Method
hfus	56.62	kJ/mol	Joback Method
hvap	93.20	kJ/mol	Joback Method
log10ws	-8.12		Crippen Method
logp	7.265		Crippen Method
mcvol	354.150	ml/mol	McGowan Method
pc	981.46	kPa	Joback Method
rinpol	2764.00		NIST Webbook
rinpol	2764.00		NIST Webbook
tb	971.21	K	Joback Method
tc	1189.13	K	Joback Method
tf	588.95	K	Joback Method
vc	1.375	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1152.28	J/mol×K	971.21	Joback Method
cpg	1167.87	J/mol×K	1007.53	Joback Method
cpg	1182.16	J/mol×K	1043.85	Joback Method
cpg	1195.19	J/mol×K	1080.17	Joback Method
cpg	1207.03	J/mol×K	1116.49	Joback Method
cpg	1217.74	J/mol×K	1152.81	Joback Method
cpg	1227.38	J/mol×K	1189.13	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=U369681&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