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

Inchi: InChI=1S/C29H46ClFO4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-23-34-27(32)29(5-2

InchiKey: GUKPVJFMCBWHKX-UHFFFAOYSA-N

Formula: C29H46ClFO4

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

Mol. weight [g/mol]: 513.12

Physical Properties

Property code	Value	Unit	Source
gf	-385.29	kJ/mol	Joback Method
hf	-1138.50	kJ/mol	Joback Method
hfus	69.57	kJ/mol	Joback Method
hvap	104.33	kJ/mol	Joback Method
log10ws	-10.21		Crippen Method
logp	9.215		Crippen Method
mcvol	424.600	ml/mol	McGowan Method
pc	741.64	kPa	Joback Method
rinpol	3297.00		NIST Webbook
rinpol	3297.00		NIST Webbook
tb	1085.61	K	Joback Method
tc	1341.38	K	Joback Method
tf	645.30	K	Joback Method
vc	1.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1463.72	J/mol×K	1085.61	Joback Method
cpg	1481.20	J/mol×K	1128.24	Joback Method
cpg	1496.89	J/mol×K	1170.87	Joback Method
cpg	1510.93	J/mol×K	1213.49	Joback Method
cpg	1523.42	J/mol×K	1256.12	Joback Method
cpg	1534.51	J/mol×K	1298.75	Joback Method
cpg	1544.30	J/mol×K	1341.38	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=U369686&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