Diethylmalonic acid, 2-fluorophenyl hexadecyl ester

Inchi: InChI=1S/C29H47FO4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-21-24-33-27(31)29(5-2,6

InchiKey: MFWJPWLMTCLSKL-UHFFFAOYSA-N

Formula: C29H47FO4

SMILES: CCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1F

Mol. weight [g/mol]: 478.68

Physical Properties

Property code	Value	Unit	Source
gf	-363.73	kJ/mol	Joback Method
hf	-1111.29	kJ/mol	Joback Method
hfus	65.76	kJ/mol	Joback Method
hvap	99.28	kJ/mol	Joback Method
log10ws	-9.53		Crippen Method
logp	8.562		Crippen Method
mcvol	412.360	ml/mol	McGowan Method
pc	763.10	kPa	Joback Method
rinpol	3113.00		NIST Webbook
rinpol	3113.00		NIST Webbook
tb	1043.20	K	Joback Method
tc	1284.86	K	Joback Method
tf	602.86	K	Joback Method
vc	1.607	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1439.51	J/mol×K	1043.20	Joback Method
cpg	1458.17	J/mol×K	1083.48	Joback Method
cpg	1475.14	J/mol×K	1123.75	Joback Method
cpg	1490.53	J/mol×K	1164.03	Joback Method
cpg	1504.44	J/mol×K	1204.30	Joback Method
cpg	1516.99	J/mol×K	1244.58	Joback Method
cpg	1528.29	J/mol×K	1284.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370140&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