Diethylmalonic acid, 2-fluorophenyl pentadecyl ester

Inchi: InChI=1S/C28H45FO4/c1-4-7-8-9-10-11-12-13-14-15-16-17-20-23-32-26(30)28(5-2,6-3)2

InchiKey: KINTWSKJBCUSDJ-UHFFFAOYSA-N

Formula: C28H45FO4

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

Mol. weight [g/mol]: 464.65

Physical Properties

Property code	Value	Unit	Source
gf	-372.15	kJ/mol	Joback Method
hf	-1090.65	kJ/mol	Joback Method
hfus	63.17	kJ/mol	Joback Method
hvap	97.06	kJ/mol	Joback Method
log10ws	-9.11		Crippen Method
logp	8.172		Crippen Method
mcvol	398.270	ml/mol	McGowan Method
pc	805.25	kPa	Joback Method
rinpol	3011.00		NIST Webbook
rinpol	3011.00		NIST Webbook
tb	1020.32	K	Joback Method
tc	1253.15	K	Joback Method
tf	591.59	K	Joback Method
vc	1.550	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1376.08	J/mol×K	1020.32	Joback Method
cpg	1394.27	J/mol×K	1059.12	Joback Method
cpg	1410.88	J/mol×K	1097.93	Joback Method
cpg	1426.00	J/mol×K	1136.73	Joback Method
cpg	1439.73	J/mol×K	1175.54	Joback Method
cpg	1452.15	J/mol×K	1214.34	Joback Method
cpg	1463.37	J/mol×K	1253.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370139&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