Diethylmalonic acid, 2-fluorophenyl octadecyl ester

Inchi: InChI=1S/C31H51FO4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-23-26-35-29(33)31
InchiKey: BMGPVJAVJDUTDB-UHFFFAOYSA-N
Formula: C31H51FO4
SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1F
Mol. weight [g/mol]: 506.73

Physical Properties

Property code	Value	Unit	Source
gf	-346.89	kJ/mol	Joback Method
hf	-1152.57	kJ/mol	Joback Method
hfus	70.94	kJ/mol	Joback Method
hvap	103.74	kJ/mol	Joback Method
log10ws	-10.37		Crippen Method
logp	9.342		Crippen Method
mcvol	440.540	ml/mol	McGowan Method
pc	688.17	kPa	Joback Method
rinpol	3315.00		NIST Webbook
rinpol	3315.00		NIST Webbook
tb	1088.96	K	Joback Method
tc	1352.40	K	Joback Method
tf	625.40	K	Joback Method
vc	1.718	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1567.38	J/mol×K	1088.96	Joback Method
cpg	1587.16	J/mol×K	1132.87	Joback Method
cpg	1604.97	J/mol×K	1176.77	Joback Method
cpg	1620.98	J/mol×K	1220.68	Joback Method
cpg	1635.35	J/mol×K	1264.59	Joback Method
cpg	1648.22	J/mol×K	1308.49	Joback Method
cpg	1659.76	J/mol×K	1352.40	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=U370142&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