Diethylmalonic acid, 4-fluoro-2-methoxyphenyl pentadecyl ester

Inchi: InChI=1S/C29H47FO5/c1-5-8-9-10-11-12-13-14-15-16-17-18-19-22-34-27(31)29(6-2,7-3
InchiKey: VBBMTMAJXSWKNZ-UHFFFAOYSA-N
Formula: C29H47FO5
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(F)cc1OC
Mol. weight [g/mol]: 494.68

Physical Properties

Property code	Value	Unit	Source
gf	-478.36	kJ/mol	Joback Method
hf	-1254.98	kJ/mol	Joback Method
hfus	66.56	kJ/mol	Joback Method
hvap	102.36	kJ/mol	Joback Method
log10ws	-9.23		Crippen Method
logp	8.181		Crippen Method
mcvol	418.230	ml/mol	McGowan Method
pc	749.79	kPa	Joback Method
rinpol	2258.00		NIST Webbook
tb	1070.60	K	Joback Method
tc	1323.26	K	Joback Method
tf	637.61	K	Joback Method
vc	1.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1467.12	J/mol×K	1070.60	Joback Method
cpg	1484.58	J/mol×K	1112.71	Joback Method
cpg	1499.96	J/mol×K	1154.82	Joback Method
cpg	1513.36	J/mol×K	1196.93	Joback Method
cpg	1524.86	J/mol×K	1239.04	Joback Method
cpg	1534.56	J/mol×K	1281.15	Joback Method
cpg	1542.55	J/mol×K	1323.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370885&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

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