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

Inchi: InChI=1S/C27H43FO5/c1-5-8-9-10-11-12-13-14-15-16-17-20-32-25(29)27(6-2,7-3)26(30

InchiKey: QEHHAQKQZXZJTC-UHFFFAOYSA-N

Formula: C27H43FO5

SMILES: CCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(F)cc1OC

Mol. weight [g/mol]: 466.63

Physical Properties

Property code	Value	Unit	Source
gf	-495.20	kJ/mol	Joback Method
hf	-1213.70	kJ/mol	Joback Method
hfus	61.38	kJ/mol	Joback Method
hvap	97.91	kJ/mol	Joback Method
log10ws	-8.39		Crippen Method
logp	7.400		Crippen Method
mcvol	390.050	ml/mol	McGowan Method
pc	835.31	kPa	Joback Method
rinpol	2971.00		NIST Webbook
tb	1024.84	K	Joback Method
tc	1258.57	K	Joback Method
tf	615.07	K	Joback Method
vc	1.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1341.44	J/mol×K	1024.84	Joback Method
cpg	1358.27	J/mol×K	1063.80	Joback Method
cpg	1373.33	J/mol×K	1102.75	Joback Method
cpg	1386.68	J/mol×K	1141.71	Joback Method
cpg	1398.40	J/mol×K	1180.66	Joback Method
cpg	1408.53	J/mol×K	1219.62	Joback Method
cpg	1417.16	J/mol×K	1258.57	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=U370890&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