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

Inchi: InChI=1S/C28H45FO5/c1-5-8-9-10-11-12-13-14-15-16-17-18-21-33-26(30)28(6-2,7-3)27

InchiKey: BQTPFRRIASFBOH-UHFFFAOYSA-N

Formula: C28H45FO5

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

Mol. weight [g/mol]: 480.65

Physical Properties

Property code	Value	Unit	Source
gf	-486.78	kJ/mol	Joback Method
hf	-1234.34	kJ/mol	Joback Method
hfus	63.97	kJ/mol	Joback Method
hvap	100.13	kJ/mol	Joback Method
log10ws	-8.81		Crippen Method
logp	7.790		Crippen Method
mcvol	404.140	ml/mol	McGowan Method
pc	790.82	kPa	Joback Method
rinpol	3068.00		NIST Webbook
rinpol	3068.00		NIST Webbook
tb	1047.72	K	Joback Method
tc	1290.25	K	Joback Method
tf	626.34	K	Joback Method
vc	1.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1404.14	J/mol×K	1047.72	Joback Method
cpg	1421.27	J/mol×K	1088.14	Joback Method
cpg	1436.49	J/mol×K	1128.56	Joback Method
cpg	1449.87	J/mol×K	1168.98	Joback Method
cpg	1461.49	J/mol×K	1209.40	Joback Method
cpg	1471.43	J/mol×K	1249.82	Joback Method
cpg	1479.77	J/mol×K	1290.25	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370891&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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