Diethylmalonic acid, 2-fluorophenyl tridecyl ester

Inchi: InChI=1S/C26H41FO4/c1-4-7-8-9-10-11-12-13-14-15-18-21-30-24(28)26(5-2,6-3)25(29)3

InchiKey: HOPHDCGQDBXZTF-UHFFFAOYSA-N

Formula: C26H41FO4

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

Mol. weight [g/mol]: 436.60

Physical Properties

Property code	Value	Unit	Source
gf	-388.99	kJ/mol	Joback Method
hf	-1049.37	kJ/mol	Joback Method
hfus	57.99	kJ/mol	Joback Method
hvap	92.61	kJ/mol	Joback Method
log10ws	-8.27		Crippen Method
logp	7.392		Crippen Method
mcvol	370.090	ml/mol	McGowan Method
pc	900.72	kPa	Joback Method
rinpol	2780.00		NIST Webbook
rinpol	2780.00		NIST Webbook
tb	974.56	K	Joback Method
tc	1193.39	K	Joback Method
tf	569.05	K	Joback Method
vc	1.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1250.41	J/mol×K	974.56	Joback Method
cpg	1267.82	J/mol×K	1011.03	Joback Method
cpg	1283.82	J/mol×K	1047.50	Joback Method
cpg	1298.48	J/mol×K	1083.97	Joback Method
cpg	1311.88	J/mol×K	1120.45	Joback Method
cpg	1324.08	J/mol×K	1156.92	Joback Method
cpg	1335.17	J/mol×K	1193.39	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=U370137&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