Diethylmalonic acid, 2-fluoro-3-trifluoromethylphenyl tridecyl ester

Inchi: InChI=1S/C27H40F4O4/c1-4-7-8-9-10-11-12-13-14-15-16-20-34-24(32)26(5-2,6-3)25(33

InchiKey: WAKCJPXSRIWIFU-UHFFFAOYSA-N

Formula: C27H40F4O4

SMILES: CCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 504.60

Physical Properties

Property code	Value	Unit	Source
gf	-971.79	kJ/mol	Joback Method
hf	-1678.56	kJ/mol	Joback Method
hfus	62.01	kJ/mol	Joback Method
hvap	91.75	kJ/mol	Joback Method
log10ws	-9.38		Crippen Method
logp	8.411		Crippen Method
mcvol	389.490	ml/mol	McGowan Method
pc	789.49	kPa	Joback Method
rinpol	2685.00		NIST Webbook
rinpol	2685.00		NIST Webbook
tb	997.00	K	Joback Method
tc	1225.89	K	Joback Method
tf	597.03	K	Joback Method
vc	1.538	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1332.50	J/mol×K	997.00	Joback Method
cpg	1350.05	J/mol×K	1035.15	Joback Method
cpg	1366.20	J/mol×K	1073.30	Joback Method
cpg	1381.04	J/mol×K	1111.44	Joback Method
cpg	1394.68	J/mol×K	1149.59	Joback Method
cpg	1407.24	J/mol×K	1187.74	Joback Method
cpg	1418.82	J/mol×K	1225.89	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=U370718&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

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