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

Inchi: InChI=1S/C29H44F4O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-22-36-26(34)28(5-2,6-3
InchiKey: OKUBNZVEUITHNJ-UHFFFAOYSA-N
Formula: C29H44F4O4
SMILES: CCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cccc(C(F)(F)F)c1F
Mol. weight [g/mol]: 532.65

Physical Properties

Property code	Value	Unit	Source
gf	-954.95	kJ/mol	Joback Method
hf	-1719.84	kJ/mol	Joback Method
hfus	67.19	kJ/mol	Joback Method
hvap	96.20	kJ/mol	Joback Method
log10ws	-10.21		Crippen Method
logp	9.191		Crippen Method
mcvol	417.670	ml/mol	McGowan Method
pc	710.73	kPa	Joback Method
rinpol	2884.00		NIST Webbook
rinpol	2884.00		NIST Webbook
tb	1042.76	K	Joback Method
tc	1291.54	K	Joback Method
tf	619.57	K	Joback Method
vc	1.649	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1458.37	J/mol×K	1042.76	Joback Method
cpg	1477.20	J/mol×K	1084.22	Joback Method
cpg	1494.41	J/mol×K	1125.69	Joback Method
cpg	1510.16	J/mol×K	1167.15	Joback Method
cpg	1524.60	J/mol×K	1208.61	Joback Method
cpg	1537.88	J/mol×K	1250.08	Joback Method
cpg	1550.14	J/mol×K	1291.54	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=U370720&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