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

Inchi: InChI=1S/C32H50F4O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-25-39-29(37)3
InchiKey: FFOAIPWGOBCYMF-UHFFFAOYSA-N
Formula: C32H50F4O4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cccc(C(F)(F)F)c1F
Mol. weight [g/mol]: 574.73

Physical Properties

Property code	Value	Unit	Source
gf	-929.69	kJ/mol	Joback Method
hf	-1781.76	kJ/mol	Joback Method
hfus	74.97	kJ/mol	Joback Method
hvap	102.88	kJ/mol	Joback Method
log10ws	-11.47		Crippen Method
logp	10.361		Crippen Method
mcvol	459.940	ml/mol	McGowan Method
pc	612.99	kPa	Joback Method
rinpol	3200.00		NIST Webbook
tb	1111.40	K	Joback Method
tc	1401.24	K	Joback Method
tf	653.38	K	Joback Method
vc	1.817	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1650.10	J/mol×K	1111.40	Joback Method
cpg	1671.42	J/mol×K	1159.71	Joback Method
cpg	1690.74	J/mol×K	1208.01	Joback Method
cpg	1708.31	J/mol×K	1256.32	Joback Method
cpg	1724.41	J/mol×K	1304.63	Joback Method
cpg	1739.29	J/mol×K	1352.94	Joback Method
cpg	1753.20	J/mol×K	1401.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370723&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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