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

Inchi: InChI=1S/C31H48F4O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-24-38-28(36)30(5
InchiKey: TXCRMBUUATWLFF-UHFFFAOYSA-N
Formula: C31H48F4O4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cccc(C(F)(F)F)c1F
Mol. weight [g/mol]: 560.70

Physical Properties

Property code	Value	Unit	Source
gf	-938.11	kJ/mol	Joback Method
hf	-1761.12	kJ/mol	Joback Method
hfus	72.38	kJ/mol	Joback Method
hvap	100.65	kJ/mol	Joback Method
log10ws	-11.05		Crippen Method
logp	9.971		Crippen Method
mcvol	445.850	ml/mol	McGowan Method
pc	643.20	kPa	Joback Method
rinpol	3098.00		NIST Webbook
rinpol	3098.00		NIST Webbook
tb	1088.52	K	Joback Method
tc	1363.02	K	Joback Method
tf	642.11	K	Joback Method
vc	1.762	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1585.84	J/mol×K	1088.52	Joback Method
cpg	1606.23	J/mol×K	1134.27	Joback Method
cpg	1624.77	J/mol×K	1180.02	Joback Method
cpg	1641.67	J/mol×K	1225.77	Joback Method
cpg	1657.13	J/mol×K	1271.52	Joback Method
cpg	1671.37	J/mol×K	1317.27	Joback Method
cpg	1684.62	J/mol×K	1363.02	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370722&Units=SI

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