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

Inchi: InChI=1S/C30H46F4O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-23-37-27(35)29(5-2,
InchiKey: CRKPUWGWNIKFPI-UHFFFAOYSA-N
Formula: C30H46F4O4
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cccc(C(F)(F)F)c1F
Mol. weight [g/mol]: 546.68

Physical Properties

Property code	Value	Unit	Source
gf	-946.53	kJ/mol	Joback Method
hf	-1740.48	kJ/mol	Joback Method
hfus	69.78	kJ/mol	Joback Method
hvap	98.43	kJ/mol	Joback Method
log10ws	-10.63		Crippen Method
logp	9.581		Crippen Method
mcvol	431.760	ml/mol	McGowan Method
pc	675.70	kPa	Joback Method
rinpol	2998.00		NIST Webbook
rinpol	2998.00		NIST Webbook
tb	1065.64	K	Joback Method
tc	1326.49	K	Joback Method
tf	630.84	K	Joback Method
vc	1.706	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1521.92	J/mol×K	1065.64	Joback Method
cpg	1541.49	J/mol×K	1109.12	Joback Method
cpg	1559.33	J/mol×K	1152.59	Joback Method
cpg	1575.62	J/mol×K	1196.07	Joback Method
cpg	1590.53	J/mol×K	1239.54	Joback Method
cpg	1604.25	J/mol×K	1283.02	Joback Method
cpg	1616.96	J/mol×K	1326.49	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=U370721&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