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

Inchi: InChI=1S/C28H42F4O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21-35-25(33)27(2,3)26
InchiKey: HRPAOWTVRUBWTD-UHFFFAOYSA-N
Formula: C28H42F4O4
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1cccc(C(F)(F)F)c1F
Mol. weight [g/mol]: 518.62

Physical Properties

Property code	Value	Unit	Source
gf	-963.37	kJ/mol	Joback Method
hf	-1699.20	kJ/mol	Joback Method
hfus	64.60	kJ/mol	Joback Method
hvap	93.97	kJ/mol	Joback Method
log10ws	-9.79		Crippen Method
logp	8.801		Crippen Method
mcvol	403.580	ml/mol	McGowan Method
pc	748.56	kPa	Joback Method
rinpol	2807.00		NIST Webbook
rinpol	2807.00		NIST Webbook
tb	1019.88	K	Joback Method
tc	1258.04	K	Joback Method
tf	608.30	K	Joback Method
vc	1.593	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1395.22	J/mol×K	1019.88	Joback Method
cpg	1413.38	J/mol×K	1059.57	Joback Method
cpg	1430.03	J/mol×K	1099.27	Joback Method
cpg	1445.30	J/mol×K	1138.96	Joback Method
cpg	1459.32	J/mol×K	1178.65	Joback Method
cpg	1472.21	J/mol×K	1218.34	Joback Method
cpg	1484.10	J/mol×K	1258.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U362008&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