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

Inchi: InChI=1S/C26H38F4O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-19-33-23(31)25(2,3)24(32)34
InchiKey: USWRWCZNOOHFTR-UHFFFAOYSA-N
Formula: C26H38F4O4
SMILES: CCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1cccc(C(F)(F)F)c1F
Mol. weight [g/mol]: 490.57

Physical Properties

Property code	Value	Unit	Source
gf	-980.21	kJ/mol	Joback Method
hf	-1657.92	kJ/mol	Joback Method
hfus	59.42	kJ/mol	Joback Method
hvap	89.52	kJ/mol	Joback Method
log10ws	-8.96		Crippen Method
logp	8.020		Crippen Method
mcvol	375.400	ml/mol	McGowan Method
pc	833.86	kPa	Joback Method
rinpol	2621.00		NIST Webbook
tb	974.12	K	Joback Method
tc	1194.98	K	Joback Method
tf	585.76	K	Joback Method
vc	1.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1270.24	J/mol×K	974.12	Joback Method
cpg	1287.25	J/mol×K	1010.93	Joback Method
cpg	1302.94	J/mol×K	1047.74	Joback Method
cpg	1317.39	J/mol×K	1084.55	Joback Method
cpg	1330.70	J/mol×K	1121.36	Joback Method
cpg	1342.97	J/mol×K	1158.17	Joback Method
cpg	1354.28	J/mol×K	1194.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U362006&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