Dimethylmalonic acid, heptadecyl 2,3,4-trifluorophenyl ester

Inchi: InChI=1S/C28H43F3O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21-34-26(32)28(2,3
InchiKey: CNTUBCYAEAGROR-UHFFFAOYSA-N
Formula: C28H43F3O4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1ccc(F)c(F)c1F
Mol. weight [g/mol]: 500.63

Physical Properties

Property code	Value	Unit	Source
gf	-781.03	kJ/mol	Joback Method
hf	-1505.81	kJ/mol	Joback Method
hfus	68.55	kJ/mol	Joback Method
hvap	96.75	kJ/mol	Joback Method
log10ws	-9.77		Crippen Method
logp	8.450		Crippen Method
mcvol	401.810	ml/mol	McGowan Method
pc	753.08	kPa	Joback Method
rinpol	2934.00		NIST Webbook
rinpol	2934.00		NIST Webbook
tb	1028.82	K	Joback Method
tc	1270.91	K	Joback Method
tf	617.81	K	Joback Method
vc	1.587	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1388.00	J/mol×K	1028.82	Joback Method
cpg	1406.10	J/mol×K	1069.17	Joback Method
cpg	1422.44	J/mol×K	1109.52	Joback Method
cpg	1437.11	J/mol×K	1149.87	Joback Method
cpg	1450.20	J/mol×K	1190.21	Joback Method
cpg	1461.80	J/mol×K	1230.56	Joback Method
cpg	1472.01	J/mol×K	1270.91	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=U361895&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