Diethylmalonic acid, 2,3,4-trifluorophenyl undecyl ester

Inchi: InChI=1S/C24H35F3O4/c1-4-7-8-9-10-11-12-13-14-17-30-22(28)24(5-2,6-3)23(29)31-19
InchiKey: GEYLNOQRPBJUQB-UHFFFAOYSA-N
Formula: C24H35F3O4
SMILES: CCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(F)c(F)c1F
Mol. weight [g/mol]: 444.53

Physical Properties

Property code	Value	Unit	Source
gf	-814.71	kJ/mol	Joback Method
hf	-1423.25	kJ/mol	Joback Method
hfus	58.19	kJ/mol	Joback Method
hvap	87.84	kJ/mol	Joback Method
log10ws	-8.10		Crippen Method
logp	6.890		Crippen Method
mcvol	345.450	ml/mol	McGowan Method
pc	940.95	kPa	Joback Method
rinpol	2487.00		NIST Webbook
tb	937.30	K	Joback Method
tc	1147.65	K	Joback Method
tf	572.73	K	Joback Method
vc	1.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1139.37	J/mol×K	937.30	Joback Method
cpg	1155.66	J/mol×K	972.36	Joback Method
cpg	1170.65	J/mol×K	1007.42	Joback Method
cpg	1184.38	J/mol×K	1042.48	Joback Method
cpg	1196.90	J/mol×K	1077.54	Joback Method
cpg	1208.27	J/mol×K	1112.59	Joback Method
cpg	1218.52	J/mol×K	1147.65	Joback Method

Sources

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=U370696&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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