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

Inchi: InChI=1S/C29H45F3O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-22-35-27(33)29(5-2,
InchiKey: COEFQQGAWMDYPQ-UHFFFAOYSA-N
Formula: C29H45F3O4
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(F)c(F)c1F
Mol. weight [g/mol]: 514.66

Physical Properties

Property code	Value	Unit	Source
gf	-772.61	kJ/mol	Joback Method
hf	-1526.45	kJ/mol	Joback Method
hfus	71.14	kJ/mol	Joback Method
hvap	98.97	kJ/mol	Joback Method
log10ws	-10.19		Crippen Method
logp	8.840		Crippen Method
mcvol	415.900	ml/mol	McGowan Method
pc	714.92	kPa	Joback Method
rinpol	3013.00		NIST Webbook
rinpol	3013.00		NIST Webbook
tb	1051.70	K	Joback Method
tc	1304.96	K	Joback Method
tf	629.08	K	Joback Method
vc	1.643	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1451.16	J/mol×K	1051.70	Joback Method
cpg	1469.82	J/mol×K	1093.91	Joback Method
cpg	1486.55	J/mol×K	1136.12	Joback Method
cpg	1501.47	J/mol×K	1178.33	Joback Method
cpg	1514.69	J/mol×K	1220.54	Joback Method
cpg	1526.32	J/mol×K	1262.75	Joback Method
cpg	1536.48	J/mol×K	1304.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370701&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