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

Inchi: InChI=1S/C30H47F3O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-23-36-28(34)30(5
InchiKey: DOUJCGGCVAQDPE-UHFFFAOYSA-N
Formula: C30H47F3O4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(F)c(F)c1F
Mol. weight [g/mol]: 528.69

Physical Properties

Property code	Value	Unit	Source
gf	-764.19	kJ/mol	Joback Method
hf	-1547.09	kJ/mol	Joback Method
hfus	73.73	kJ/mol	Joback Method
hvap	101.20	kJ/mol	Joback Method
log10ws	-10.61		Crippen Method
logp	9.230		Crippen Method
mcvol	429.990	ml/mol	McGowan Method
pc	679.58	kPa	Joback Method
rinpol	3117.00		NIST Webbook
rinpol	3117.00		NIST Webbook
tb	1074.58	K	Joback Method
tc	1340.50	K	Joback Method
tf	640.35	K	Joback Method
vc	1.698	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1514.64	J/mol×K	1074.58	Joback Method
cpg	1533.90	J/mol×K	1118.90	Joback Method
cpg	1551.05	J/mol×K	1163.22	Joback Method
cpg	1566.23	J/mol×K	1207.54	Joback Method
cpg	1579.58	J/mol×K	1251.86	Joback Method
cpg	1591.23	J/mol×K	1296.18	Joback Method
cpg	1601.32	J/mol×K	1340.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370702&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