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

Inchi: InChI=1S/C25H37F3O4/c1-4-7-8-9-10-11-12-13-14-15-18-31-23(29)25(5-2,6-3)24(30)32

InchiKey: KIRMRXVJJZSKBJ-UHFFFAOYSA-N

Formula: C25H37F3O4

SMILES: CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(F)c(F)c1F

Mol. weight [g/mol]: 458.55

Physical Properties

Property code	Value	Unit	Source
gf	-806.29	kJ/mol	Joback Method
hf	-1443.89	kJ/mol	Joback Method
hfus	60.78	kJ/mol	Joback Method
hvap	90.07	kJ/mol	Joback Method
log10ws	-8.52		Crippen Method
logp	7.280		Crippen Method
mcvol	359.540	ml/mol	McGowan Method
pc	887.88	kPa	Joback Method
rinpol	2580.00		NIST Webbook
rinpol	2580.00		NIST Webbook
tb	960.18	K	Joback Method
tc	1176.72	K	Joback Method
tf	584.00	K	Joback Method
vc	1.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1200.84	J/mol×K	960.18	Joback Method
cpg	1217.53	J/mol×K	996.27	Joback Method
cpg	1232.82	J/mol×K	1032.36	Joback Method
cpg	1246.78	J/mol×K	1068.45	Joback Method
cpg	1259.45	J/mol×K	1104.54	Joback Method
cpg	1270.89	J/mol×K	1140.63	Joback Method
cpg	1281.16	J/mol×K	1176.72	Joback Method

Sources

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=U370697&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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