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

Inchi: InChI=1S/C26H39F3O4/c1-4-7-8-9-10-11-12-13-14-15-16-19-32-24(30)26(5-2,6-3)25(31)

InchiKey: OVTFTJLRWYIEHN-UHFFFAOYSA-N

Formula: C26H39F3O4

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

Mol. weight [g/mol]: 472.58

Physical Properties

Property code	Value	Unit	Source
gf	-797.87	kJ/mol	Joback Method
hf	-1464.53	kJ/mol	Joback Method
hfus	63.37	kJ/mol	Joback Method
hvap	92.30	kJ/mol	Joback Method
log10ws	-8.94		Crippen Method
logp	7.670		Crippen Method
mcvol	373.630	ml/mol	McGowan Method
pc	839.19	kPa	Joback Method
rinpol	2702.00		NIST Webbook
rinpol	2702.00		NIST Webbook
tb	983.06	K	Joback Method
tc	1206.89	K	Joback Method
tf	595.27	K	Joback Method
vc	1.474	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1262.80	J/mol×K	983.06	Joback Method
cpg	1279.92	J/mol×K	1020.36	Joback Method
cpg	1295.54	J/mol×K	1057.67	Joback Method
cpg	1309.72	J/mol×K	1094.97	Joback Method
cpg	1322.54	J/mol×K	1132.28	Joback Method
cpg	1334.04	J/mol×K	1169.58	Joback Method
cpg	1344.31	J/mol×K	1206.89	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=U370698&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