Diethylmalonic acid, 3,4-difluorobenzyl tridecyl ester

Inchi: InChI=1S/C27H42F2O4/c1-4-7-8-9-10-11-12-13-14-15-16-19-32-25(30)27(5-2,6-3)26(31)
InchiKey: ZTTPVNVAIXKJDD-UHFFFAOYSA-N
Formula: C27H42F2O4
SMILES: CCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCc1ccc(F)c(F)c1
Mol. weight [g/mol]: 468.62

Physical Properties

Property code	Value	Unit	Source
gf	-585.01	kJ/mol	Joback Method
hf	-1277.59	kJ/mol	Joback Method
hfus	63.27	kJ/mol	Joback Method
hvap	94.68	kJ/mol	Joback Method
log10ws	-8.87		Crippen Method
logp	7.669		Crippen Method
mcvol	385.950	ml/mol	McGowan Method
pc	821.95	kPa	Joback Method
rinpol	2848.00		NIST Webbook
rinpol	2848.00		NIST Webbook
tb	1001.69	K	Joback Method
tc	1230.01	K	Joback Method
tf	593.43	K	Joback Method
vc	1.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1319.15	J/mol×K	1001.69	Joback Method
cpg	1336.80	J/mol×K	1039.74	Joback Method
cpg	1352.91	J/mol×K	1077.80	Joback Method
cpg	1367.55	J/mol×K	1115.85	Joback Method
cpg	1380.80	J/mol×K	1153.90	Joback Method
cpg	1392.74	J/mol×K	1191.96	Joback Method
cpg	1403.45	J/mol×K	1230.01	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369333&Units=SI

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