Diethylmalonic acid, 3,4-difluorobenzyl undecyl ester

Inchi: InChI=1S/C25H38F2O4/c1-4-7-8-9-10-11-12-13-14-17-30-23(28)25(5-2,6-3)24(29)31-19
InchiKey: YCGQUGOAGWHWSB-UHFFFAOYSA-N
Formula: C25H38F2O4
SMILES: CCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCc1ccc(F)c(F)c1
Mol. weight [g/mol]: 440.56

Physical Properties

Property code	Value	Unit	Source
gf	-601.85	kJ/mol	Joback Method
hf	-1236.31	kJ/mol	Joback Method
hfus	58.09	kJ/mol	Joback Method
hvap	90.23	kJ/mol	Joback Method
log10ws	-8.03		Crippen Method
logp	6.888		Crippen Method
mcvol	357.770	ml/mol	McGowan Method
pc	920.50	kPa	Joback Method
rinpol	2644.00		NIST Webbook
rinpol	2644.00		NIST Webbook
tb	955.93	K	Joback Method
tc	1170.52	K	Joback Method
tf	570.89	K	Joback Method
vc	1.401	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1194.57	J/mol×K	955.93	Joback Method
cpg	1211.43	J/mol×K	991.69	Joback Method
cpg	1226.92	J/mol×K	1027.46	Joback Method
cpg	1241.11	J/mol×K	1063.22	Joback Method
cpg	1254.07	J/mol×K	1098.99	Joback Method
cpg	1265.84	J/mol×K	1134.75	Joback Method
cpg	1276.49	J/mol×K	1170.52	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=U369331&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

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