Diethylmalonic acid, 3,4-difluorobenzyl dodecyl ester

Inchi: InChI=1S/C26H40F2O4/c1-4-7-8-9-10-11-12-13-14-15-18-31-24(29)26(5-2,6-3)25(30)32
InchiKey: WXPAJBBHOZKPHJ-UHFFFAOYSA-N
Formula: C26H40F2O4
SMILES: CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCc1ccc(F)c(F)c1
Mol. weight [g/mol]: 454.59

Physical Properties

Property code	Value	Unit	Source
gf	-593.43	kJ/mol	Joback Method
hf	-1256.95	kJ/mol	Joback Method
hfus	60.68	kJ/mol	Joback Method
hvap	92.45	kJ/mol	Joback Method
log10ws	-8.45		Crippen Method
logp	7.279		Crippen Method
mcvol	371.860	ml/mol	McGowan Method
pc	869.14	kPa	Joback Method
rinpol	2746.00		NIST Webbook
rinpol	2746.00		NIST Webbook
tb	978.81	K	Joback Method
tc	1199.70	K	Joback Method
tf	582.16	K	Joback Method
vc	1.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1256.63	J/mol×K	978.81	Joback Method
cpg	1273.87	J/mol×K	1015.62	Joback Method
cpg	1289.66	J/mol×K	1052.44	Joback Method
cpg	1304.07	J/mol×K	1089.25	Joback Method
cpg	1317.16	J/mol×K	1126.07	Joback Method
cpg	1329.02	J/mol×K	1162.88	Joback Method
cpg	1339.70	J/mol×K	1199.70	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=U369332&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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