Diethylmalonic acid, 3,4-difluorobenzyl octadecyl ester

Inchi: InChI=1S/C32H52F2O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-24-37-30(35)3

InchiKey: QBBHCSVTCXGJNV-UHFFFAOYSA-N

Formula: C32H52F2O4

SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCc1ccc(F)c(F)c1

Mol. weight [g/mol]: 538.75

Physical Properties

Property code	Value	Unit	Source
gf	-542.91	kJ/mol	Joback Method
hf	-1380.79	kJ/mol	Joback Method
hfus	76.22	kJ/mol	Joback Method
hvap	105.81	kJ/mol	Joback Method
log10ws	-10.96		Crippen Method
logp	9.619		Crippen Method
mcvol	456.400	ml/mol	McGowan Method
pc	635.12	kPa	Joback Method
rinpol	3371.00		NIST Webbook
tb	1116.09	K	Joback Method
tc	1401.90	K	Joback Method
tf	649.78	K	Joback Method
vc	1.792	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1637.14	J/mol×K	1116.09	Joback Method
cpg	1657.64	J/mol×K	1163.72	Joback Method
cpg	1675.83	J/mol×K	1211.36	Joback Method
cpg	1691.91	J/mol×K	1258.99	Joback Method
cpg	1706.06	J/mol×K	1306.63	Joback Method
cpg	1718.49	J/mol×K	1354.26	Joback Method
cpg	1729.38	J/mol×K	1401.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369337&Units=SI
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

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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