Diethylmalonic acid, 3,4-difluorobenzyl hexadecyl ester

Inchi: InChI=1S/C30H48F2O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-22-35-28(33)30(5-2,

InchiKey: KKPDHHKAWLEZSP-UHFFFAOYSA-N

Formula: C30H48F2O4

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

Mol. weight [g/mol]: 510.70

Physical Properties

Property code	Value	Unit	Source
gf	-559.75	kJ/mol	Joback Method
hf	-1339.51	kJ/mol	Joback Method
hfus	71.04	kJ/mol	Joback Method
hvap	101.36	kJ/mol	Joback Method
log10ws	-10.13		Crippen Method
logp	8.839		Crippen Method
mcvol	428.220	ml/mol	McGowan Method
pc	701.35	kPa	Joback Method
rinpol	3153.00		NIST Webbook
tb	1070.33	K	Joback Method
tc	1328.66	K	Joback Method
tf	627.24	K	Joback Method
vc	1.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1509.00	J/mol×K	1070.33	Joback Method
cpg	1528.20	J/mol×K	1113.39	Joback Method
cpg	1545.45	J/mol×K	1156.44	Joback Method
cpg	1560.89	J/mol×K	1199.50	Joback Method
cpg	1574.64	J/mol×K	1242.55	Joback Method
cpg	1586.84	J/mol×K	1285.61	Joback Method
cpg	1597.63	J/mol×K	1328.66	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=U369335&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

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