Isonipecotic acid, N-(4-fluoro-2-trifluoromethylbenzoyl)-, hexadecyl ester

Inchi: InChI=1S/C30H45F4NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-22-38-29(37)24-18-20-3
InchiKey: CUUJRQFEXHYVLS-UHFFFAOYSA-N
Formula: C30H45F4NO3
SMILES: CCCCCCCCCCCCCCCCOC(=O)C1CCN(C(=O)c2ccc(F)cc2C(F)(F)F)CC1
Mol. weight [g/mol]: 543.68

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.94		Crippen Method
logp	8.721		Crippen Method
mcvol	425.010	ml/mol	McGowan Method
rinpol	3552.00		NIST Webbook
rinpol	3552.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U361256&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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