

Isonipecotic acid, N-(2-fluoro-3-trifluoromethylbenzoyl)-, tridecyl

Inchi:
ester

InChI=1S/C27H39F4NO3/c1-2-3-4-5-6-7-8-9-10-11-12-20-35-26(34)21-16-18-32(19-17-2

InchiKey:

VYJVGNJPRBRFND-UHFFFAOYSA-N

Formula:

C27H39F4NO3

SMILES:

CCCCCCCCCCCCOC(=O)C1CCN(C(=O)c2cccc(C(F)(F)F)c2F)CC1

Mol. weight [g/mol]:

501.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.68		Crippen Method
logp	7.551		Crippen Method
mcvol	382.740	ml/mol	McGowan Method
rinpole	3258.00		NIST Webbook
rinpole	3258.00		NIST Webbook

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.cheméo.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=U361319&Units=SI>

Legend

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

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