

Isonipecotic acid, N-(3-fluoro-6-trifluoromethylbenzoyl)-, decyl

Inchi:
ester

InChI=1S/C24H33F4NO3/c1-2-3-4-5-6-7-8-9-16-32-23(31)18-12-14-29(15-13-18)22(30)2

InchiKey:

VRABLHOZTZAQOF-UHFFFAOYSA-N

Formula:

C24H33F4NO3

SMILES:

CCCCCCCCCOC(=O)C1CCN(C(=O)c2cc(F)ccc2C(F)(F)F)CC1

Mol. weight [g/mol]:

459.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.43		Crippen Method
logp	6.381		Crippen Method
mcvol	340.470	ml/mol	McGowan Method
rinpola	2896.00		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=U361337&Units=SI>

Legend

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

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