

Isonipecotic acid, N-(4-fluoro-2-trifluoromethylbenzoyl)-, octyl

Inchi:
ester

InChI=1S/C22H29F4NO3/c1-2-3-4-5-6-7-14-30-21(29)16-10-12-27(13-11-16)20(28)18-9

InchiKey:

IZJKCXFCEQRNRK-UHFFFAOYSA-N

Formula:

C22H29F4NO3

SMILES:

CCCCCCCCOC(=O)C1CCN(C(=O)c2ccc(F)cc2C(F)(F)F)CC1

Mol. weight [g/mol]:

431.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.59		Crippen Method
logp	5.600		Crippen Method
mcvol	312.290	ml/mol	McGowan Method
rinsol	2690.00		NIST Webbook

Sources

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=U361248&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

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

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