

Isonipecotic acid, N-(2,4,5-trifluoro-3-methoxybenzoyl)-, octyl

InChI:
ester

InChI=1S/C22H30F3NO4/c1-3-4-5-6-7-8-13-30-22(28)15-9-11-26(12-10-15)21(27)16-14

InChIKey:

UBCKQDBRZVZZMY-UHFFFAOYSA-N

Formula:

C22H30F3NO4

SMILES:

CCCCCCCCOC(=O)C1CCN(C(=O)c2cc(F)c(F)c(OC)c2F)CC1

Mol. weight [g/mol]:

429.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.27		Crippen Method
logp	4.868		Crippen Method
mcvol	316.390	ml/mol	McGowan Method
rinpol	2945.00		NIST Webbook
rinpol	2945.00		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=U361355&Units=SI>

Crippen Method:

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

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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