

Isonipecotic acid, N-(2,5-di(trifluoromethyl)benzoyl)-, heptadecyl

Inchi:
ester

InChI=1S/C32H47F6NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-23-42-30(41)25-19-2

InchiKey:

SAHSZPVYOAGLBO-UHFFFAOYSA-N

Formula:

C32H47F6NO3

SMILES:

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

Mol. weight [g/mol]:

607.71

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.13		Crippen Method
logp	9.991		Crippen Method
mcvol	456.730	ml/mol	McGowan Method
rinpol	3480.00		NIST Webbook
rinpol	3480.00		NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U361217&Units=SI>

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>

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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