

Isonipecotic acid, N-(3-trifluoromethylbenzoyl)-, hexyl ester

Inchi: InChI=1S/C20H26F3NO3/c1-2-3-4-5-13-27-19(26)15-9-11-24(12-10-15)18(25)16-7-6-8-1
InchiKey: CRWTUSVUOCFEHF-UHFFFAOYSA-N
Formula: C20H26F3NO3
SMILES: CCCCCOC(=O)C1CCN(C(=O)c2cccc(C(F)(F)F)c2)CC1
Mol. weight [g/mol]: 385.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.42		Crippen Method
logp	4.681		Crippen Method
mcvol	282.340	ml/mol	McGowan Method
rinpola	2537.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=U361546&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

Latest version available from:

<https://www.chemeo.com/cid/54-931-8/Isonipecotic-acid-N-3-trifluoromethylbenzoyl-hexyl-ester.pdf>

Generated by Cheméo on 2024-04-26 04:33:05.80326935 +0000 UTC m=+16395234.723846672.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.