

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

Inchi: InChI=1S/C16H18F3NO3/c1-2-23-15(22)11-6-8-20(9-7-11)14(21)12-4-3-5-13(10-12)16(17)
InchiKey: QBHCDRNQQRHVRH-UHFFFAOYSA-N
Formula: C16H18F3NO3
SMILES: CCOC(=O)C1CCN(C(=O)c2cccc(C(F)(F)F)c2)CC1
Mol. weight [g/mol]: 329.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.75		Crippen Method
logp	3.121		Crippen Method
mcvol	225.980	ml/mol	McGowan Method
rinpola	2129.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361540&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/33-645-9/Isonipecotic-acid-N-3-trifluoromethylbenzoyl-ethyl-ester.pdf>

Generated by Cheméo on 2024-04-24 21:48:48.887483089 +0000 UTC m=+16284577.808060405.

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