

Isonipecotic acid, N-(2-trifluoromethylbenzoyl)-, octyl ester

Inchi: InChI=1S/C22H30F3NO3/c1-2-3-4-5-6-9-16-29-21(28)17-12-14-26(15-13-17)20(27)18-1
InchiKey: WHHBFTLXQNBYDW-UHFFFAOYSA-N
Formula: C22H30F3NO3
SMILES: CCCCCCOC(=O)C1CCN(C(=O)c2ccccc2C(F)(F)F)CC1
Mol. weight [g/mol]: 413.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.26		Crippen Method
logp	5.461		Crippen Method
mcvol	310.520	ml/mol	McGowan Method
rinpola	2780.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361493&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.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.cheméo.com/cid/32-687-4/Isonipecotic-acid-N-2-trifluoromethylbenzoyl-octyl-ester.pdf>

Generated by Cheméo on 2024-04-27 10:34:13.389838456 +0000 UTC m=+16503302.310415768.

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