

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

Inchi: InChI=1S/C20H26F3NO3/c1-2-3-4-7-14-27-19(26)15-10-12-24(13-11-15)18(25)16-8-5-6
InchiKey: YYGMGLKYKPOUGD-UHFFFAOYSA-N
Formula: C20H26F3NO3
SMILES: CCCCCCOC(=O)C1CCN(C(=O)c2ccccc2C(F)(F)F)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
rinpol	2578.00		NIST Webbook
rinpol	2578.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361491&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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
rinpol: Non-polar retention indices

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