

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

Inchi: InChI=1S/C18H22F3NO3/c1-2-3-11-25-17(24)13-7-9-22(10-8-13)16(23)14-5-4-6-15(12-1
InchiKey: FXNRKNLIJIPIDB-UHFFFAOYSA-N
Formula: C18H22F3NO3
SMILES: CCCOC(=O)C1CCN(C(=O)c2cccc(C(F)(F)F)c2)CC1
Mol. weight [g/mol]: 357.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.58		Crippen Method
logp	3.901		Crippen Method
mcvol	254.160	ml/mol	McGowan Method
rinpole	2336.00		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=U361543&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpole: Non-polar retention indices

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