

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

Inchi: InChI=1S/C17H20F3NO3/c1-2-10-24-16(23)12-6-8-21(9-7-12)15(22)13-4-3-5-14(11-13)1
InchiKey: IFUXOAYGFZDBPA-UHFFFAOYSA-N
Formula: C17H20F3NO3
SMILES: CCCOC(=O)C1CCN(C(=O)c2cccc(C(F)(F)F)c2)CC1
Mol. weight [g/mol]: 343.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.16		Crippen Method
logp	3.511		Crippen Method
mcvol	240.070	ml/mol	McGowan Method
rinpola	2233.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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=U361541&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

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