

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

Inchi: InChI=1S/C17H23NO3/c1-3-11-21-17(20)14-7-9-18(10-8-14)16(19)15-6-4-5-13(2)12-15/
InchiKey: SEKZJUGRKLIFYFG-UHFFFAOYSA-N
Formula: C17H23NO3
SMILES: CCCOC(=O)C1CCN(C(=O)c2cccc(C)c2)CC1
Mol. weight [g/mol]: 289.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.54		Crippen Method
logp	2.800		Crippen Method
mcvol	234.760	ml/mol	McGowan Method
rinpol	2443.00		NIST Webbook
rinpol	2443.00		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=U361096&Units=SI>

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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