

Isonipecotic acid, N-benzoyl-, ethyl ester

Inchi: InChI=1S/C15H19NO3/c1-2-19-15(18)13-8-10-16(11-9-13)14(17)12-6-4-3-5-7-12/h3-7,13-15
InchiKey: KZRCFZMHWBAFHJ-UHFFFAOYSA-N
Formula: C15H19NO3
SMILES: CCOC(=O)C1CCN(C(=O)c2ccccc2)CC1
Mol. weight [g/mol]: 261.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.64		Crippen Method
logp	2.102		Crippen Method
mcvol	206.580	ml/mol	McGowan Method
rinpol	2234.00		NIST Webbook
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Sources

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=U360970&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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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