

Isonipecotic acid, N-benzoyl-, pentyl ester

Inchi: InChI=1S/C18H25NO3/c1-2-3-7-14-22-18(21)16-10-12-19(13-11-16)17(20)15-8-5-4-6-9-
InchiKey: SICDZKAMSUNLAF-UHFFFAOYSA-N
Formula: C18H25NO3
SMILES: CCCCCOC(=O)C1CCN(C(=O)c2ccccc2)CC1
Mol. weight [g/mol]: 303.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.90		Crippen Method
logp	3.272		Crippen Method
mcvol	248.850	ml/mol	McGowan Method
rinpol	2564.00		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=U360974&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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