

Isonipecotic acid, N-benzoyl-, decyl ester

Inchi: InChI=1S/C23H35NO3/c1-2-3-4-5-6-7-8-12-19-27-23(26)21-15-17-24(18-16-21)22(25)20
InchiKey: NALQVVBIWDFION-UHFFFAOYSA-N
Formula: C23H35NO3
SMILES: CCCCCCCCCOC(=O)C1CCN(C(=O)c2ccccc2)CC1
Mol. weight [g/mol]: 373.53

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.99		Crippen Method
logp	5.223		Crippen Method
mcvol	319.300	ml/mol	McGowan Method
rinpol	3108.00		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=U360980&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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