Isonipecotic acid, N-benzoyl-, isohexyl ester

Inchi: InChI=1S/C19H27NO3/c1-15(2)7-6-14-23-19(22)17-10-12-20(13-11-17)18(21)16-8-4-3-5
InchiKey: YFGSSKRDTZTILS-UHFFFAOYSA-N
Formula: C19H27NO3
SMILES: CC(C)CCCOC(=O)C1CCN(C(=O)c2ccccc2)CC1
Mol. weight [g/mol]: 317.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.08		Crippen Method
logp	3.518		Crippen Method
mcvol	262.940	ml/mol	McGowan Method
rinpol	2628.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U360975&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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