

Cis-3-benzoyl-4-phenyl-1-methylpiperdine

Inchi: InChI=1S/C19H21NO/c1-20-13-11-15(12-14-20)17-9-5-6-10-18(17)19(21)16-7-3-2-4-8-1
InchiKey: SHSOBZCAJYXYSY-UHFFFAOYSA-N
Formula: C19H21NO
SMILES: CN1CCC(c2ccccc2C(=O)c2ccccc2)CC1
Mol. weight [g/mol]: 279.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.34		Crippen Method
logp	3.727		Crippen Method
mcvol	231.740	ml/mol	McGowan Method

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=B6003516&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

Latest version available from:

<https://www.chemeo.com/cid/82-144-1/Cis-3-benzoyl-4-phenyl-1-methylpiperdine.pdf>

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