

# Trans-3-benzoyl-4-phenyl-1-methylpiperdine

<b>Inchi:</b>	InChI=1S/C19H21NO/c1-20-13-12-17(15-8-4-2-5-9-15)18(14-20)19(21)16-10-6-3-7-11-1
<b>InchiKey:</b>	XYCHMYKPKLTNDM-UHFFFAOYSA-N
<b>Formula:</b>	C19H21NO
<b>SMILES:</b>	CN1CCC(c2ccccc2)C(C(=O)c2ccccc2)C1
<b>Mol. weight [g/mol]:</b>	279.38
<b>CAS:</b>	116595-02-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.03		Crippen Method
logp	3.605		Crippen Method
mcvol	231.740	ml/mol	McGowan Method

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C116595029&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116595029&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume

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