

Piperazine,1-benzyl-4-(2-pyridyl)-

Inchi:	InChI=1S/C16H19N3/c1-2-6-15(7-3-1)14-18-10-12-19(13-11-18)16-8-4-5-9-17-16/h1-9H,
InchiKey:	PPZUTXLPTNQOFF-UHFFFAOYSA-N
Formula:	C16H19N3
SMILES:	c1ccc(CN2CCN(c3ccccc3)CC2)cc1
Mol. weight [g/mol]:	253.34
CAS:	63980-42-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.98		Crippen Method
logp	2.404		Crippen Method
mcvol	207.860	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C63980427&Units=SI

Legend

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

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<https://www.chemeo.com/cid/82-252-1/Piperazine-1-benzyl-4-2-pyridyl.pdf>

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