

1-Benzylpiperazine

Other names:	N-Benzylpiperazine
	Piperazine, 1-(phenylmethyl)-
	Benzylpiperazine
	Piperazine, 1-benzyl-
	4-Benzylpiperazine
	BZP
	N-(Phenylmethyl)piperazine
Inchi:	InChI=1S/C11H16N2/c1-2-4-11(5-3-1)10-13-8-6-12-7-9-13/h1-5,12H,6-10H2
InchiKey:	IQXXEPZFOOTTBA-UHFFFAOYSA-N
Formula:	C11H16N2
SMILES:	<chem>c1ccc(CN2CCNCC2)cc1</chem>
Mol. weight [g/mol]:	176.26
CAS:	2759-28-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.68		Crippen Method
logp	1.092		Crippen Method
mcvol	151.190	ml/mol	McGowan Method
rinpol	1516.10		NIST Webbook

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=C2759286&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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