

Piperazine, n,n'-diphenyl-

Other names:	1,4-diphenylpiperazine
Inchi:	InChI=1S/C16H18N2/c1-3-7-15(8-4-1)17-11-13-18(14-12-17)16-9-5-2-6-10-16/h1-10H,11
InchiKey:	LLZRSOPHIGKISM-UHFFFAOYSA-N
Formula:	C16H18N2
SMILES:	<chem>c1ccc(N2CCN(c3ccccc3)CC2)cc1</chem>
Mol. weight [g/mol]:	238.33
CAS:	613-39-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.83		Crippen Method
logp	3.013		Crippen Method
mcvol	197.880	ml/mol	McGowan Method
tf	437.15 ± 2.00	K	NIST Webbook

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=C613398&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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<https://www.chemeo.com/cid/43-322-6/Piperazine-n-n-diphenyl.pdf>

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