

2,3-Diphenylpyrazine

Inchi:	InChI=1S/C16H12N2/c1-3-7-13(8-4-1)15-16(18-12-11-17-15)14-9-5-2-6-10-14/h1-12H
InchiKey:	PTZIVVDMBCVSMR-UHFFFAOYSA-N
Formula:	C16H12N2
SMILES:	c1ccc(-c2nccnc2-c2ccccc2)cc1
Mol. weight [g/mol]:	232.28
CAS:	1588-89-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.21		Crippen Method
logp	3.811		Crippen Method
mcvol	184.980	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1588892&Units=SI
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

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/15-445-1/2-3-Diphenylpyrazine.pdf>

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