

2-(P-n-pentylanilino)-3-methyl pyrazine

Inchi:	InChI=1S/C16H21N3/c1-3-4-5-6-14-7-9-15(10-8-14)19-16-13(2)17-11-12-18-16/h7-12H,3
InchiKey:	MFNGZKMUPMOGCW-UHFFFAOYSA-N
Formula:	C16H21N3
SMILES:	CCCCCc1ccc(N=c2[nH]ccnc2C)cc1
Mol. weight [g/mol]:	255.36
CAS:	116660-50-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.45		Crippen Method
logp	3.201		Crippen Method
mcvol	218.720	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=C116660505&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/82-392-6/2-P-n-pentylanilino-3-methyl-pyrazine.pdf>

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