

2-(P-pentylanilino)-3,6-dimethyl pyrazine

Inchi:	InChI=1S/C17H23N3/c1-4-5-6-7-15-8-10-16(11-9-15)20-17-14(3)18-12-13(2)19-17/h8-12
InchiKey:	ULUAFBQRAKARCG-UHFFFAOYSA-N
Formula:	C17H23N3
SMILES:	CCCCCc1ccc(N=c2[nH]c(C)cnc2C)cc1
Mol. weight [g/mol]:	269.38
CAS:	116660-23-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.92		Crippen Method
logp	3.510		Crippen Method
mcvol	232.810	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C116660232&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/82-994-8/2-P-pentylanilino-3-6-dimethyl-pyrazine.pdf>

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