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