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/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=C116660505&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume