

2-(P-t-dodecylanilino)-3-methyl pyrazine

Inchi:	InChI=1S/C23H35N3/c1-5-6-7-8-9-10-11-16-23(3,4)20-12-14-21(15-13-20)26-22-19(2)24
InchiKey:	GKBAEGMOHNLNKJ-UHFFFAOYSA-N
Formula:	C23H35N3
SMILES:	CCCCCCCCC(C)(C)c1ccc(Nc2nccnc2C)cc1
Mol. weight [g/mol]:	353.54
CAS:	116402-82-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.95		Crippen Method
logp	6.947		Crippen Method
mcvol	317.350	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=C116402825&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/56-655-3/2-P-t-dodecylanilino-3-methyl-pyrazine.pdf>

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