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: CCCCCCCCCC(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/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=C116402825&Units=SI

Legend

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