2-(N-methylanilino)-3-tridecyl pyrazine

Inchi: InChI=1S/C24H37N3/c1-3-4-5-6-7-8-9-10-11-12-16-19-23-24(26-21-20-25-23)27(2)22-17
InchiKey: ZOLISYGBANSINI-UHFFFAOYSA-N
Formula: C24H37N3
SMILES: CCCCCCCCCCCCCc1nccnc1N(C)c1ccccc1
Mol. weight [g/mol]: 367.57
CAS: 116402-91-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.12		Crippen Method
logp	7.098		Crippen Method
mcvol	331.440	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=C116402916&Units=SI

Legend

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