

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)c1cccc1
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

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<https://www.chemeo.com/cid/86-752-2/2-N-methylanilino-3-tridecyl-pyrazine.pdf>

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