

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

Inchi:	InChI=1S/C18H17N3/c1-21(16-10-6-3-7-11-16)18-17(19-12-13-20-18)14-15-8-4-2-5-9-15
InchiKey:	JIXAVCAMURZTSK-UHFFFAOYSA-N
Formula:	C18H17N3
SMILES:	CN(c1ccccc1)c1nccnc1Cc1ccccc1
Mol. weight [g/mol]:	275.35
CAS:	116660-02-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.81		Crippen Method
logp	3.835		Crippen Method
mcvol	223.140	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=C116660027&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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