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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116660027&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume