

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

Inchi:	InChI=1S/C19H19N3/c1-22(17-10-6-3-7-11-17)19-18(20-14-15-21-19)13-12-16-8-4-2-5-9
InchiKey:	CLILIRTUKVJUOF-UHFFFAOYSA-N
Formula:	C19H19N3
SMILES:	CN(c1ccccc1)c1nccnc1CCc1ccccc1
Mol. weight [g/mol]:	289.37
CAS:	116659-75-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.13		Crippen Method
logp	4.030		Crippen Method
mcvol	237.230	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=C116659757&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/82-089-3/2-N-methylanilino-3-2-phenylethyl-pyrazine.pdf>

Generated by Cheméo on 2024-04-18 08:09:29.832764494 +0000 UTC m=+15717018.753341810.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.