

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

Inchi:	InChI=1S/C12H13N3/c1-10-12(14-9-8-13-10)15(2)11-6-4-3-5-7-11/h3-9H,1-2H3
InchiKey:	MVNJTWHIQSTKKM-UHFFFAOYSA-N
Formula:	C12H13N3
SMILES:	Cc1nccnc1N(C)c1ccccc1
Mol. weight [g/mol]:	199.25
CAS:	88613-84-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.18		Crippen Method
logp	2.553		Crippen Method
mcvol	162.360	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=C88613847&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

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