

3-(N-methylanilino)-2-methyl-5-(n-heptyl)pyrazine

Inchi:	InChI=1S/C19H27N3/c1-4-5-6-7-9-12-17-15-20-16(2)19(21-17)22(3)18-13-10-8-11-14-18
InchiKey:	BSHFCHHHZJOO-UHFFFAOYSA-N
Formula:	C19H27N3
SMILES:	CCCCCCCc1cnc(C)c(N(C)c2cccc2)n1
Mol. weight [g/mol]:	297.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.08		Crippen Method
logp	5.066		Crippen Method
mcvol	260.990	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6002659&Units=SI
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

Legend

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

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