

3-(N-methylanilino)-2-methyl-5-(5-nonyl)pyrazine

Inchi:	InChI=1S/C21H31N3/c1-5-7-12-18(13-8-6-2)20-16-22-17(3)21(23-20)24(4)19-14-10-9-11
InchiKey:	BHYFJUZVMGGTBL-UHFFFAOYSA-N
Formula:	C21H31N3
SMILES:	CCCCC(CCCC)c1cnc(C)c(N(C)c2cccc2)n1
Mol. weight [g/mol]:	325.49
CAS:	116660-08-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.88		Crippen Method
logp	6.017		Crippen Method
mcvol	289.170	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116660083&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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