

2-(N-methylanilino)-6-(5-nonyl) pyrazine

Inchi:	InChI=1S/C20H29N3/c1-4-6-11-17(12-7-5-2)19-15-21-16-20(22-19)23(3)18-13-9-8-10-14
InchiKey:	OHQIPGUAYZNHIR-UHFFFAOYSA-N
Formula:	C20H29N3
SMILES:	CCCCC(CCCC)c1cncc(N(C)c2ccccc2)n1
Mol. weight [g/mol]:	311.46
CAS:	116660-11-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.40		Crippen Method
logp	5.708		Crippen Method
mcvol	275.080	ml/mol	McGowan Method

Sources

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=C116660118&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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