

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

Inchi: InChI=1S/C20H29N3/c1-4-6-11-17(12-7-5-2)19-20(22-16-15-21-19)23(3)18-13-9-8-10-14
InchiKey: IYQJHOAIKVGRDB-UHFFFAOYSA-N
Formula: C20H29N3
SMILES: CCCCC(CCCC)c1nccnc1N(C)c1cccc1
Mol. weight [g/mol]: 311.46
CAS: 116660-10-7

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: <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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C116660107&Units=SI>

Legend

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

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