

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

InChI: InChI=1S/C25H39N3/c1-5-8-12-19-23-25(28(4)22-17-13-11-14-18-22)27-24(20-26-23)21(15-9-6-2)16-10-7-3/h11,13-14,17-18,20-21H,5-10,12,15-16,19H2,1-4H3

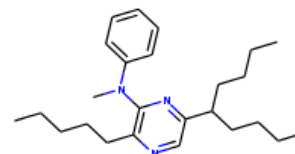
InChI Key: MRRFTOZE BMVKNW-UHFFFAOYSA-N

Formula: C₂₅H₃₉N₃

SMILES: CCCCCc1ncc(C(CCCC)CCCC)nc1N(C)c1cccc1

Molecular Weight: 381.60

CAS: 116402-97-2



Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	7.441		Crippen Method

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C25H39N3/c1-5-8-12-19-23-25\(28\(4\)22-17-13-11-14-18-22\)27-24\(20-26-23\)21\(15-9-6-2\)16-10-7-3/h11,13-14,17-18,20-21H,5-10,12,15-16,19H2,1-4H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C25H39N3/c1-5-8-12-19-23-25(28(4)22-17-13-11-14-18-22)27-24(20-26-23)21(15-9-6-2)16-10-7-3/h11,13-14,17-18,20-21H,5-10,12,15-16,19H2,1-4H3)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

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