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)c2ccccc2)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

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=C116660083&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume