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
InchiKey: MRRFTOZEBMVKNW-UHFFFAOYSA-N
Formula: C25H39N3
SMILES: CCCCCc1ncc(C(CCCC)CCCC)nc1N(C)c1ccccc1
Mol. weight [g/mol]: 381.60
CAS: 116402-97-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.46		Crippen Method
logp	7.441		Crippen Method
mcvol	345.530	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=C116402972&Units=SI

Legend

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