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

Inchi: InChI=1S/C23H35N3/c1-4-6-8-9-12-15-20-19-24-22(18-11-7-5-2)23(25-20)26(3)21-16-13

InchiKey: QFNYGBRCCGYZQK-UHFFFAOYSA-N

Formula: C23H35N3

SMILES: CCCCCCCc1cnc(CCCCC)c(N(C)c2ccccc2)n1

Mol. weight [g/mol]: 353.54

CAS: 116402-85-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.66		Crippen Method
logp	6.490		Crippen Method
mcvol	317.350	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402858&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume