2-(N-methylanilino)-3-(n-hexyl) pyrazine

Inchi: InChI=1S/C17H23N3/c1-3-4-5-9-12-16-17(19-14-13-18-16)20(2)15-10-7-6-8-11-15/h6-8,
InchiKey: DIPCNSVVYPMWDR-UHFFFAOYSA-N
Formula: C17H23N3
SMILES: CCCCCCc1nccnc1N(C)c1ccccc1
Mol. weight [g/mol]: 269.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.18		Crippen Method
logp	4.367		Crippen Method
mcvol	232.810	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=B6002792&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