2-(N-methylanilino)-3-(2-phenylethyl) pyrazine

Inchi: InChI=1S/C19H19N3/c1-22(17-10-6-3-7-11-17)19-18(20-14-15-21-19)13-12-16-8-4-2-5-9

InchiKey: CLILIRTUKVJUOF-UHFFFAOYSA-N

Formula: C19H19N3

SMILES: CN(c1ccccc1)c1nccnc1CCc1ccccc1

Mol. weight [g/mol]: 289.37

CAS: 116659-75-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.13		Crippen Method
logp	4.030		Crippen Method
mcvol	237.230	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=C116659757&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume