2-(N-methylanilino)-3-(p-phenoxybenzyl) pyrazine

Inchi: InChI=1S/C24H21N3O/c1-27(20-8-4-2-5-9-20)24-23(25-16-17-26-24)18-19-12-14-22(15-

InchiKey: ZDBGSDDVWFJTQI-UHFFFAOYSA-N

Formula: C24H21N3O

SMILES: CN(c1ccccc1)c1nccnc1Cc1ccc(Oc2ccccc2)cc1

Mol. weight [g/mol]: 367.44

CAS: 116659-76-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.44		Crippen Method
logp	5.628		Crippen Method
mcvol	289.790	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116659768&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