

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(15-16)
InchiKey: ZDBGSDDVWFJTQI-UHFFFAOYSA-N
Formula: C24H21N3O
SMILES: CN(c1cccc1)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/ci9903071>
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

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