2-(M-phenoxyanilino)-3-methyl pyrazine

Inchi: InChI=1S/C17H15N3O/c1-13-17(19-11-10-18-13)20-14-6-5-9-16(12-14)21-15-7-3-2-4-8-
InchiKey: MBEOHGZQIBJQOX-UHFFFAOYSA-N
Formula: C17H15N3O
SMILES: Cc1nccnc1Nc1cccc(Oc2ccccc2)c1
Mol. weight [g/mol]: 277.32
CAS: 116659-74-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.92		Crippen Method
logp	4.321		Crippen Method
mcvol	214.920	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=C116659746&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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