

2-(O-phenylphenoxy)-3-methyl pyrazine

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|-----------------------------|----------------------------------------------------------------------------------|
| Inchi: | InChI=1S/C17H14N2O/c1-13-17(19-12-11-18-13)20-16-10-6-5-9-15(16)14-7-3-2-4-8-14/ |
| InchiKey: | USLZXOBENXPOCF-UHFFFAOYSA-N |
| Formula: | C17H14N2O |
| SMILES: | Cc1nccnc1Oc1ccccc1-c1ccccc1 |
| Mol. weight [g/mol]: | 262.31 |
| CAS: | 93323-45-6 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -5.72 | | Crippen Method |
| logp | 4.244 | | Crippen Method |
| mcvol | 204.940 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C93323456&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

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

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