

# 2-(P-nonylphenoxy) pyrazine

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C19H26N2O/c1-2-3-4-5-6-7-8-9-17-10-12-18(13-11-17)22-19-16-20-14-15-21- |
| <b>InchiKey:</b>            | PGRRFTMMIQTILZ-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C19H26N2O  |
| <b>SMILES:</b>              | CCCCCCCCc1ccc(Oc2cnccn2)cc1  |
| <b>Mol. weight [g/mol]:</b> | 298.42   |
| <b>CAS:</b>                 | 116659-78-0  |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -6.37   |        | Crippen Method |
| logp          | 5.562   |        | Crippen Method |
| mcvol         | 256.880 | ml/mol | McGowan Method |

## Sources

|                        |   |
|------------------------|---|
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                           |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C116659780&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116659780&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                       |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                               |

## Legend

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

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