

2-(P-dodecylphenoxy) pyrazine

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|-----------------------------|--|
| Inchi: | InChI=1S/C22H32N2O/c1-2-3-4-5-6-7-8-9-10-11-12-20-13-15-21(16-14-20)25-22-19-23- |
| InchiKey: | MLOJPIGVCAHKEM-UHFFFAOYSA-N |
| Formula: | C22H32N2O |
| SMILES: | CCCCCCCCCCCCc1ccc(Oc2cnccn2)cc1 |
| Mol. weight [g/mol]: | 340.50 |
| CAS: | 116660-31-2 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -7.63 | | Crippen Method |
| logp | 6.732 | | Crippen Method |
| mcvol | 299.150 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C116660312&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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<https://www.chemeo.com/cid/84-459-0/2-P-dodecylphenoxy-pyrazine.pdf>

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