

2-(P-nonylphenoxy)-3-methyl-6-benzyl pyrazine

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|-----------------------------|--|
| Inchi: | InChI=1S/C27H34N2O/c1-3-4-5-6-7-8-10-13-23-16-18-26(19-17-23)30-27-22(2)28-21-25 |
| InchiKey: | BERFGWOXHRCHLZ-UHFFFAOYSA-N |
| Formula: | C27H34N2O |
| SMILES: | CCCCCCCCc1ccc(Oc2nc(Cc3ccccc3)cnc2C)cc1 |
| Mol. weight [g/mol]: | 402.57 |
| CAS: | 116402-76-7 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -8.95 | | Crippen Method |
| logp | 7.461 | | Crippen Method |
| mcvol | 345.840 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402767&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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