

2-(P-nonylphenoxy)-3-(p-phenoxybenzyl)pyrazine

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|-----------------------------|--|
| Inchi: | InChI=1S/C32H36N2O2/c1-2-3-4-5-6-7-9-12-26-15-19-30(20-16-26)36-32-31(33-23-24-3 |
| InchiKey: | QHGGSDYGTUIUPI-UHFFFAOYSA-N |
| Formula: | C32H36N2O2 |
| SMILES: | CCCCCCCCc1ccc(Oc2nccnc2Cc2ccc(Oc3ccccc3)cc2)cc1 |
| Mol. weight [g/mol]: | 480.64 |
| CAS: | 116402-78-9 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -10.11 | | Crippen Method |
| logp | 8.945 | | Crippen Method |
| mcvol | 398.400 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|---|
| 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 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402789&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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