

4-(2-Phenoxyphenyl) morpholine

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|-----------------------------|--|
| Inchi: | InChI=1S/C16H17NO2/c1-2-6-14(7-3-1)19-16-9-5-4-8-15(16)17-10-12-18-13-11-17/h1-9 |
| InchiKey: | KVMSYYSWHAELLX-UHFFFAOYSA-N |
| Formula: | C16H17NO2 |
| SMILES: | c1ccc(Oc2ccccc2N2CCOCC2)cc1 |
| Mol. weight [g/mol]: | 255.31 |
| CAS: | 116400-68-1 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -2.83 | | Crippen Method |
| logp | 3.315 | | Crippen Method |
| mcvol | 199.640 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|---|
| 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=C116400681&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/40-046-6/4-2-Phenoxyphenyl-morpholine.pdf>

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