

2-(P-t-butylphenoxy)-3-methyl pyrazine

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|-----------------------------|--|
| Inchi: | InChI=1S/C15H18N2O/c1-11-14(17-10-9-16-11)18-13-7-5-12(6-8-13)15(2,3)4/h5-10H,1- |
| InchiKey: | QSRWVAHHWVLRU-UHFFFAOYSA-N |
| Formula: | C15H18N2O |
| SMILES: | Cc1nccnc1Oc1ccc(C(C)(C)C)cc1 |
| Mol. weight [g/mol]: | 242.32 |
| CAS: | 116660-14-1 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -4.43 | | Crippen Method |
| logp | 3.875 | | Crippen Method |
| mcvol | 200.520 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C116660141&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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