

# 2-Phenoxy-3-tridecyl pyrazine

|                      |                                                                                  |
|----------------------|----------------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C23H34N2O/c1-2-3-4-5-6-7-8-9-10-11-15-18-22-23(25-20-19-24-22)26-21-16- |
| InchiKey:            | DDJCJUNERJIMJL-UHFFFAOYSA-N                                                      |
| Formula:             | C23H34N2O                                                                        |
| SMILES:              | CCCCCCCCCCCCCc1nccnc1Oc1ccccc1                                                   |
| Mol. weight [g/mol]: | 354.53                                                                           |
| CAS:                 | 116659-46-2                                                                      |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -8.05   |        | Crippen Method |
| logp          | 7.122   |        | Crippen Method |
| mcvol         | 313.240 | ml/mol | McGowan Method |

## Sources

|                 |                                                                                                                                                 |
|-----------------|-------------------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                               |
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                           |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C116659462&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116659462&amp;Units=SI</a> |
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                       |

## 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/13-740-5/2-Phenoxy-3-tridecyl-pyrazine.pdf>

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