# 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:** 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=C116659462&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