

# 2-Phenoxy pyrazine

**Other names:** Phenoxy pyrazine  
Pyrazine, phenoxy-

**Inchi:** InChI=1S/C10H8N2O/c1-2-4-9(5-3-1)13-10-8-11-6-7-12-10/h1-8H

**InchiKey:** LKXUZLSVURTETC-UHFFFAOYSA-N

**Formula:** C10H8N2O

**SMILES:** c1ccc(Oc2cnccn2)cc1

**Mol. weight [g/mol]:** 172.18

**CAS:** 107697-82-5

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -2.64   |        | Crippen Method |
| logp          | 2.269   |        | Crippen Method |
| mcvol         | 130.070 | ml/mol | McGowan Method |
| rinpol        | 1415.00 |        | NIST Webbook   |
| rinpol        | 1415.00 |        | NIST Webbook   |
| ripol         | 2104.00 |        | NIST Webbook   |

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C107697825&Units=SI>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## Legend

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume

**rinpol:** Non-polar retention indices

**ripol:** Polar retention indices

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