

1-(p-Nitrophenyl)pyrrole

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|-----------------------------|--|
| Other names: | 1-(4-nitrophenyl)pyrrole |
| Inchi: | InChI=1S/C10H8N2O2/c13-12(14)10-5-3-9(4-6-10)11-7-1-2-8-11/h1-8H |
| InchiKey: | PWCFKNYSCGRNRW-UHFFFAOYSA-N |
| Formula: | C10H8N2O2 |
| SMILES: | O=[N+](O-)c1ccc(-n2cccc2)cc1 |
| Mol. weight [g/mol]: | 188.18 |
| CAS: | 4533-42-0 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -3.77 | | Crippen Method |
| logp | 2.385 | | Crippen Method |
| mcvol | 135.940 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|---|
| 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 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C4533420&Units=SI |

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/118-134-2/1-p-Nitrophenyl-pyrrole.pdf>

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