

Pyrrolidine, 1-nitroso-

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| Other names: | N-Nitrosopyrrolidine 1-Nitrosopyrrolidine N-Nitrosopyrrolidin Nitrosopyrrolidine No-Pyr NPYR 1-Pyrrolidinamine, N-nitroso- |
| Inchi: | InChI=1S/C4H8N2O/c7-5-6-3-1-2-4-6/h1-4H2 |
| InchiKey: | WNYADZVDBIBLJJ-UHFFFAOYSA-N |
| Formula: | C4H8N2O |
| SMILES: | O=NN1CCCC1 |
| Mol. weight [g/mol]: | 100.12 |
| CAS: | 930-55-2 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|--------|--------|----------------|
| log10ws | -1.14 | | Crippen Method |
| logp | 0.764 | | Crippen Method |
| mcvol | 77.890 | ml/mol | McGowan Method |
| rinpol | 952.00 | | NIST Webbook |
| rinpol | 175.18 | | NIST Webbook |
| rinpol | 176.52 | | NIST Webbook |
| tb | 487.20 | K | NIST Webbook |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C930552&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

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|-----------------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| rinpol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |

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<https://www.cheméo.com/cid/41-931-2/Pyrrolidine-1-nitroso.pdf>

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