

2-Amino-4-phenyl oxazole

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|-----------------------------|---|
| Inchi: | InChI=1S/C9H8N2O/c10-9-11-8(6-12-9)7-4-2-1-3-5-7/h1-6H,(H2,10,11) |
| InchiKey: | FXRWCCOADRNYMB-UHFFFAOYSA-N |
| Formula: | C9H8N2O |
| SMILES: | <chem>Nc1nc(-c2ccccc2)co1</chem> |
| Mol. weight [g/mol]: | 160.17 |
| CAS: | 33119-65-2 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -7.21 | | Crippen Method |
| logp | 1.924 | | Crippen Method |
| mcvol | 120.280 | 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=C33119652&Units=SI |

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/67-006-1/2-Amino-4-phenyl-oxazole.pdf>

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