

4-Amino-1-phenylpyrazolo(3,4-e)pyrimidine

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|-----------------------------|---|
| Inchi: | InChI=1S/C11H9N5/c12-10-9-6-15-16(11(9)14-7-13-10)8-4-2-1-3-5-8/h1-7H,(H2,12,13,14) |
| InchiKey: | KKDPIZPUTYIBFX-UHFFFAOYSA-N |
| Formula: | C11H9N5 |
| SMILES: | Nc1ncnc2c1cnn2-c1ccccc1 |
| Mol. weight [g/mol]: | 211.22 |
| CAS: | 5334-30-5 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -3.86 | | Crippen Method |
| logp | 1.398 | | Crippen Method |
| mcvol | 153.070 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| 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=C5334305&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/17-603-3/4-Amino-1-phenylpyrazolo-3-4-e-pyrimidine.pdf>

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