

Imidazole, 5-amino-4-pyrrolidinylcarbonyl-

| | |
|-----------------------------|---|
| Inchi: | InChI=1S/C8H12N4O/c9-7-6(10-5-11-7)8(13)12-3-1-2-4-12/h5H,1-4,9H2,(H,10,11) |
| InchiKey: | BCTKLWHOWGYBFD-UHFFFAOYSA-N |
| Formula: | C8H12N4O |
| SMILES: | <chem>Nc1[nH]cnc1C(=O)N1CCCC1</chem> |
| Mol. weight [g/mol]: | 180.21 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -0.97 | | Crippen Method |
| logp | -0.254 | | Crippen Method |
| mcvol | 134.750 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|---|
| 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=B6010456&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

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/65-435-7/Imidazole-5-amino-4-pyrrolidinylcarbonyl.pdf>

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