

3-Pyridinecarboxylic acid, 6-amino-

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|-----------------------------|--|
| Other names: | Nicotinic acid, 6-amino- 2-Amino-5-pyridinecarboxylic acid 6-Aminonicotinic acid |
| Inchi: | InChI=1S/C6H6N2O2/c7-5-2-1-4(3-8-5)6(9)10/h1-3H,(H2,7,8)(H,9,10) |
| InchiKey: | ZCIFWRHIEBXBOY-UHFFFAOYSA-N |
| Formula: | C6H6N2O2 |
| SMILES: | <chem>Nc1ccc(C(=O)O)cn1</chem> |
| Mol. weight [g/mol]: | 138.12 |
| CAS: | 3167-49-5 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|--------|--------|----------------|
| log10ws | -0.93 | | Crippen Method |
| logp | 0.362 | | Crippen Method |
| mcvol | 99.040 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C3167495&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

| | |
|-----------------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |

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