

Aziridine, 1-phenyl-

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|-----------------------------|--|
| Other names: | N-Phenylaziridine N-Phenylethylenimine 1-Phenylaziridine |
| Inchi: | InChI=1S/C8H9N/c1-2-4-8(5-3-1)9-6-7-9/h1-5H,6-7H2 |
| InchiKey: | YKNKBBMRKMLLJS-UHFFFAOYSA-N |
| Formula: | C8H9N |
| SMILES: | <chem>c1ccc(N2CC2)cc1</chem> |
| Mol. weight [g/mol]: | 119.16 |
| CAS: | 696-18-4 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|-------------|--------|----------------|
| affp | 926.50 | kJ/mol | NIST Webbook |
| basg | 895.70 | kJ/mol | NIST Webbook |
| ie | 8.00 ± 0.10 | eV | NIST Webbook |
| ie | 8.19 ± 0.06 | eV | NIST Webbook |
| ie | 8.10 | eV | NIST Webbook |
| ie | 8.00 | eV | NIST Webbook |
| log10ws | -1.27 | | Crippen Method |
| logp | 1.507 | | Crippen Method |
| mcvol | 98.940 | 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=C696184&Units=SI |

Legend

| | |
|-----------------|-------------------------------------|
| affp: | Proton affinity |
| basg: | Gas basicity |
| ie: | Ionization energy |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |

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