

# 1-Azabicyclo[2.2.2]octan-3-one

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | 3-Quinuclidinone<br>3-Oxoquinuclidine<br>3-Quinuclidone<br>MKC-2<br>Quinuclidone 3<br>Quinuclidin-3-one<br>NSC 168448 |
| <b>Inchi:</b>               | InChI=1S/C7H11NO/c9-7-5-8-3-1-6(7)2-4-8/h6H,1-5H2   |
| <b>InchiKey:</b>            | ZKMZPXWMMMSBLNO-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C7H11NO   |
| <b>SMILES:</b>              | O=C1CN2CCC1CC2  |
| <b>Mol. weight [g/mol]:</b> | 125.17  |
| <b>CAS:</b>                 | 3731-38-2   |

## Physical Properties

| Property code | Value  | Unit   | Source         |
|---------------|--------|--------|----------------|
| affp          | 936.00 | kJ/mol | NIST Webbook   |
| basg          | 905.20 | kJ/mol | NIST Webbook   |
| ie            | 8.20   | eV     | NIST Webbook   |
| log10ws       | -0.15  |        | Crippen Method |
| logp          | 0.281  |        | Crippen Method |
| mcvol         | 99.320 | ml/mol | McGowan Method |

## Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                   |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                           |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                       |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C3731382&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3731382&amp;Units=SI</a> |

# Legend

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

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