

# 1H-Indole-3-carboxaldehyde

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | Indole-3-carboxaldehyde<br>«beta»-Indolylaldehyde<br>Indol-3-carboxaldehyde<br>Indole-3-aldehyde<br>Indole-3-carbaldehyde<br>3-Formylindole<br>3-Indolealdehyde<br>3-Indolecarbaldehyde<br>3-Indolecarboxaldehyde<br>Indole-3-carboxyaldehyde<br>beta-Indolylaldehyde<br>1H-Indole-3-carbaldehyde<br>Indol-3-carbaldehyde<br>1H-Indole-3-aldehyde<br>NSC 10118 |
| <b>Inchi:</b>               | InChI=1S/C9H7NO/c11-6-7-5-10-9-4-2-1-3-8(7)9/h1-6,10H  |
| <b>InchiKey:</b>            | OLNJUISKUQQNIM-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C9H7NO   |
| <b>SMILES:</b>              | O=Cc1c[nH]c2ccccc12  |
| <b>Mol. weight [g/mol]:</b> | 145.16   |
| <b>CAS:</b>                 | 487-89-8   |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -2.74   |        | Crippen Method |
| logp          | 1.498   |        | Crippen Method |
| mcvol         | 110.300 | ml/mol | McGowan Method |
| rinpol        | 1816.10 |        | NIST Webbook   |
| rinpol        | 1816.10 |        | NIST Webbook   |

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C487898&Units=SI>

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:**

[https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)

## Legend

|                 |                                     |
|-----------------|-------------------------------------|
| <b>log10ws:</b> | Log10 of Water solubility in mol/l  |
| <b>logp:</b>    | Octanol/Water partition coefficient |
| <b>mcvol:</b>   | McGowan's characteristic volume     |
| <b>rinpol:</b>  | Non-polar retention indices         |

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