

1H-Indole-4-carboxaldehyde

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|-----------------------------|---|
| Other names: | Indole-4-carboxaldehyde 1H-Indole-4-carbaldehyde |
| Inchi: | InChI=1S/C9H7NO/c11-6-7-2-1-3-9-8(7)4-5-10-9/h1-6,10H |
| InchiKey: | JFDDDFGLNZWNJTK-UHFFFAOYSA-N |
| Formula: | C9H7NO |
| SMILES: | O=Cc1cccc2[nH]ccc12 |
| Mol. weight [g/mol]: | 145.16 |
| CAS: | 1074-86-8 |

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 | 1717.50 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| 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=C1074868&Units=SI |

Legend

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

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