

# Indoleacetic acid

|                     |   |
|---------------------|---|
| <b>Other names:</b> | (1H-Indol-3-yl)-acetic acid<br>1H-Indole-3-acetic acid<br>2-(1H-indol-3-yl)acetic acid<br>2-(1H-indol-3-yl)ethanoic acid<br>2-(3-Indolyl)acetic acid<br>3-(Carboxymethyl)Indole<br>3-IAA<br>3-Indoleacetic acid<br>3-Indolylacetic acid<br>Acetic acid, indolyl-<br>GAP<br>Heteroauxin<br>Heteroauxine<br>Heteroauxinhexteroauxiniae<br>Hexteroauxin<br>IAA<br>Indol-3-ylacetic acid<br>Indole-3-acetic acid<br>Indolyl-3-acetic acid<br>Indolylacetic acid<br>Kyselina 3-indolyloctova<br>NSC 3787<br>Rhizopin<br>Rhizopon A<br>«alpha»-IAA<br>«alpha»-Indol-3-yl-acetic acid<br>«beta»-IAA<br>«beta»-Indole-3-acetic acid<br>«beta»-Indoleacetic acid<br>«beta»-Indolylacetic acid<br>«omega»-Skatole carboxylic acid<br>Â«alphaÂ»-IAA<br>Â«alphaÂ»-Indol-3-yl-acetic acid<br>Â«betaÂ»-IAA<br>Â«betaÂ»-Indole-3-acetic acid<br>Â«betaÂ»-Indoleacetic acid<br>Â«betaÂ»-Indolylacetic acid<br>Â«omegaÂ»-Skatole carboxylic acid |
| <b>Inchi:</b>       | InChI=1S/C10H9NO2/c12-10(13)5-7-6-11-9-4-2-1-3-8(7)9/h1-4,6,11H,5H2,(H,12,13)   |
| <b>InchiKey:</b>    | SEOVTRFCIGRIMH-UHFFFAOYSA-N   |

**Formula:** C10H8NO2  
**SMILES:** O=C(O)Cc1c[nH]c2ccccc12  
**Mol. weight [g/mol]:** 174.18  
**CAS:** 87-51-4

## Physical Properties

| Property code | Value   | Unit   | Source                               |
|---------------|---------|--------|--------------------------------------|
| log10ws       | -2.05   |        | Aqueous Solubility Prediction Method |
| logp          | 1.313   |        | Crippen Method                       |
| mvol          | 130.260 | ml/mol | McGowan Method                       |
| tf            | 441.65  | K      | Aqueous Solubility Prediction Method |

## Temperature Dependent Properties

| Property code | Value        | Unit   | Temperature [K] | Source       |
|---------------|--------------|--------|-----------------|--------------|
| hsubt         | 64.00 ± 1.50 | kJ/mol | 368.00          | NIST Webbook |

## Sources

|   |   |
|---|---|
| <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=C87514&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C87514&amp;Units=SI</a>   |
| <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>Equilibrium Solubility, Model Correlation, and Solvent Effect of Aqueous Solubility Prediction Method:</b> | <a href="https://www.doi.org/10.1021/acs.jced.8b01265">https://www.doi.org/10.1021/acs.jced.8b01265</a>   |
| <b>Solvents:</b>  | <a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx</a> |

## Legend

|                 |  |
|-----------------|--|
| <b>hsubt:</b>   | Enthalpy of sublimation at a given temperature |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l             |
| <b>logp:</b>    | Octanol/Water partition coefficient            |

**mcvol:** McGowan's characteristic volume

**tf:** Normal melting (fusion) point

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