

# 1H-Indole-3-acetic acid, ethyl ester

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | Indole-3-acetic acid, ethyl ester<br>Ethyl «beta»-indolylacetate<br>Ethyl indol-3-ylacetate<br>Ethyl indole-3-acetate<br>Ethyl 3-indoleacetate<br>Ethyl 3-indolylacetate<br>Ethyl 1H-indol-3-ylacetate<br>NSC 38002<br>3-Indoleacetic acid, ethyl ester |
| <b>Inchi:</b>               | InChI=1S/C12H13NO2/c1-2-15-12(14)7-9-8-13-11-6-4-3-5-10(9)11/h3-6,8,13H,2,7H2,1H  |
| <b>InchiKey:</b>            | HUDBDWIQSIGUDI-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C12H13NO2   |
| <b>SMILES:</b>              | CCOC(=O)Cc1c[nH]c2ccccc12   |
| <b>Mol. weight [g/mol]:</b> | 203.24  |
| <b>CAS:</b>                 | 778-82-5  |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -3.00   |        | Crippen Method |
| logp          | 1.792   |        | Crippen Method |
| mcvol         | 158.440 | ml/mol | McGowan Method |
| rinpol        | 1903.00 |        | NIST Webbook   |
| rinpol        | 1903.00 |        | NIST Webbook   |

## Pressure Dependent Properties

| Property code | Value  | Unit | Pressure [kPa] | Source       |
|---------------|--------|------|----------------|--------------|
| tbrp          | 438.20 | K    | 0.10           | NIST Webbook |

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C778825&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307I>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpol:** Non-polar retention indices  
**tbrp:** Boiling point at reduced pressure

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