

# Indole-2-carboxylic acid

|                      |                                                                                                                           |
|----------------------|---------------------------------------------------------------------------------------------------------------------------|
| Other names:         | 1H-indole-2-carboxylic acid<br>2-Indolecarboxylic acid<br>2-carboxyindole<br>2-indolylformic acid<br>indole-2-formic acid |
| Inchi:               | InChI=1S/C9H7NO2/c11-9(12)8-5-6-3-1-2-4-7(6)10-8/h1-5,10H,(H,11,12)                                                       |
| InchiKey:            | HCUARRIEZVDMPT-UHFFFAOYSA-N                                                                                               |
| Formula:             | C9H7NO2                                                                                                                   |
| SMILES:              | O=C(O)c1cc2ccccc2[nH]1                                                                                                    |
| Mol. weight [g/mol]: | 161.16                                                                                                                    |
| CAS:                 | 1477-50-5                                                                                                                 |

## Physical Properties

| Property code | Value   | Unit   | Source                                                                                                   |
|---------------|---------|--------|----------------------------------------------------------------------------------------------------------|
| log10ws       | -2.56   |        | Crippen Method                                                                                           |
| logp          | 1.384   |        | Crippen Method                                                                                           |
| mcvol         | 116.170 | ml/mol | McGowan Method                                                                                           |
| tf            | 483.10  | K      | Experimental and computational thermochemical study of benzofuran, benzothiophene and indole derivatives |

## Sources

|                                                                                                           |                                                                                                                                             |
|-----------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method:                                                                                           | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                   |
| Crippen Method:                                                                                           | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                           |
| Experimental and computational thermochemical study of benzofuran, benzothiophene and indole derivatives: | <a href="https://www.doi.org/10.1016/j.jct.2016.02.008">https://www.doi.org/10.1016/j.jct.2016.02.008</a>                                   |
| Measurement and Correlation of Solubilities of Indole-2-carboxylic Acid                                   | <a href="https://www.doi.org/10.1021/je400813d">https://www.doi.org/10.1021/je400813d</a>                                                   |
| McGowan Method                                                                                            | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                       |
| McGowan Method                                                                                            | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1477505&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1477505&amp;Units=SI</a> |
| (278.15 to 360.15) K:                                                                                     |                                                                                                                                             |
| NIST Webbook:                                                                                             |                                                                                                                                             |

# 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>tf:</b>      | Normal melting (fusion) point       |

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