

# 3-Carboxaldehyde, 5-methylindole-

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C10H9NO/c1-7-2-3-10-9(4-7)8(6-12)5-11-10/h2-6,11H,1H3 |
| <b>InchiKey:</b>            | ZTNQWTPWKNDRNF-UHFFFAOYSA-N                                    |
| <b>Formula:</b>             | C10H9NO  |
| <b>SMILES:</b>              | <chem>Cc1ccc2[nH]cc(C=O)c2c1</chem>                            |
| <b>Mol. weight [g/mol]:</b> | 159.18   |
| <b>CAS:</b>                 | 52562-50-2   |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -3.21   |        | Crippen Method |
| logp          | 1.807   |        | Crippen Method |
| mcvol         | 124.390 | ml/mol | McGowan Method |

## Sources

|                        |   |
|------------------------|---|
| <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>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                             |
| <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=C52562502&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C52562502&amp;Units=SI</a> |

## 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     |

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