

# 1-(Fur-2-ylmethyl)-2-formyl-pyrrole

|                      |                                                                                                                                                              |
|----------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | 1-furfuryl-2-formylpyrrole<br>1-(2-furanylmethyl)-2-formyl- 1H-pyrrole<br>1-(2-furfuryl)pyrrole-2-carboxaldehyde<br>Pyrrole-2-carboxaldehyde, 1-(2-furfuryl) |
| Inchi:               | InChI=1S/C10H9NO2/c12-8-9-3-1-5-11(9)7-10-4-2-6-13-10/h1-6,8H,7H2                                                                                            |
| InchiKey:            | PYBJPTHZYBWJON-UHFFFAOYSA-N                                                                                                                                  |
| Formula:             | C10H9NO2                                                                                                                                                     |
| SMILES:              | O=Cc1cccn1Cc1ccco1                                                                                                                                           |
| Mol. weight [g/mol]: | 175.18                                                                                                                                                       |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -7.01   |        | Crippen Method |
| logp          | 1.942   |        | Crippen Method |
| mcvol         | 130.260 | ml/mol | McGowan Method |
| rinpol        | 1374.00 |        | NIST Webbook   |
| rinpol        | 1374.00 |        | NIST Webbook   |
| rinpol        | 1384.00 |        | NIST Webbook   |
| ripol         | 2254.00 |        | NIST Webbook   |
| ripol         | 2266.00 |        | NIST Webbook   |
| ripol         | 2266.00 |        | NIST Webbook   |
| ripol         | 2254.00 |        | NIST Webbook   |

## Sources

|                 |                                                                                                                                         |
|-----------------|-----------------------------------------------------------------------------------------------------------------------------------------|
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                   |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R87946&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R87946&amp;Units=SI</a> |
| 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>                       |

# 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>rinpol:</b>  | Non-polar retention indices         |
| <b>ripol:</b>   | Polar retention indices             |

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