

# 3-ACETAMIDOFURAN

|                             |                                                         |
|-----------------------------|---------------------------------------------------------|
| <b>Inchi:</b>               | InChI=1S/C6H7NO2/c1-5(8)7-6-2-3-9-4-6/h2-4H,1H3,(H,7,8) |
| <b>InchiKey:</b>            | MSUYGSATOVDCFI-UHFFFAOYSA-N                             |
| <b>Formula:</b>             | C6H7NO2                                                 |
| <b>SMILES:</b>              | CC(=O)Nc1ccoc1                                          |
| <b>Mol. weight [g/mol]:</b> | 125.13                                                  |

## Physical Properties

| Property code | Value   | Unit   | Source             |
|---------------|---------|--------|--------------------|
| ie            | 8.57    | eV     | Cheméo Relay (1.0) |
| log10ws       | -0.75   |        | Cheméo Relay (1.0) |
| logp          | 1.238   |        | Crippen Method     |
| mcvol         | 93.360  | ml/mol | McGowan Method     |
| rinpol        | 1202.00 |        | NIST Webbook       |
| rinpol        | 1202.00 |        | NIST Webbook       |
| tb            | 503.30  | K      | Cheméo Relay (1.0) |
| tf            | 334.75  | K      | Cheméo Relay (1.0) |

## Sources

|                                  |                                                                                                                                               |
|----------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| <b>NIST Webbook:</b>             | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C59445851&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C59445851&amp;Units=SI</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>Crippen Method:</b>           | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>Cheméo Relay (1.0):</b>       |                                                                                                                                               |
| <b>Cheméo Relay (1.0, beta):</b> |                                                                                                                                               |

## Legend

|                 |                                     |
|-----------------|-------------------------------------|
| <b>ie:</b>      | Ionization energy                   |
| <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>tb:</b>     | Normal Boiling Point Temperature |
| <b>tf:</b>     | Normal melting (fusion) point    |

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