

# Pyrrole, 1-acetyl

|                      |                                              |
|----------------------|----------------------------------------------|
| Other names:         | Pyrrole, 1-acetyl                            |
| Inchi:               | InChI=1S/C6H7NO/c1-6(8)7-4-2-3-5-7/h2-5H,1H3 |
| InchiKey:            | OMYOJDLCFAUIHN-UHFFFAOYSA-N                  |
| Formula:             | C6H7NO                                       |
| SMILES:              | CC(=O)n1cccc1                                |
| Mol. weight [g/mol]: | 109.13                                       |

## Physical Properties

| Property code | Value   | Unit   | Source             |
|---------------|---------|--------|--------------------|
| ie            | 9.21    | eV     | Cheméo Relay (1.0) |
| logp          | 1.148   |        | Crippen Method     |
| mcvol         | 87.490  | ml/mol | McGowan Method     |
| rinpol        | 948.00  |        | NIST Webbook       |
| rinpol        | 957.00  |        | NIST Webbook       |
| ripol         | 1554.00 |        | NIST Webbook       |
| ripol         | 1576.00 |        | NIST Webbook       |

## Sources

|                           |                                                                                                                                           |
|---------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| McGowan Method:           | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| 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>                         |
| Cheméo Relay (1.0):       |                                                                                                                                           |
| Cheméo Relay (1.0, beta): |                                                                                                                                           |
| NIST Webbook:             | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C609416&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C609416&amp;Units=SI</a> |

## Legend

|        |                                     |
|--------|-------------------------------------|
| ie:    | Ionization energy                   |
| logp:  | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume     |

**rinpol:** Non-polar retention indices

**ripol:** Polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/65-100-8/Pyrrole-1-acetyl.pdf>

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