

# 2-Acetylpyrazine

|                      |                                                 |
|----------------------|-------------------------------------------------|
| Other names:         | acetylpyrazine<br>pyrazine, acetyl-             |
| Inchi:               | InChI=1S/C6H6N2O/c1-5(9)6-4-7-2-3-8-6/h2-4H,1H3 |
| InchiKey:            | DBZAKQWXICEWNW-UHFFFAOYSA-N                     |
| Formula:             | C6H6N2O                                         |
| SMILES:              | CC(=O)c1cnccn1                                  |
| Mol. weight [g/mol]: | 122.12                                          |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -1.66   |        | Crippen Method |
| logp          | 0.679   |        | Crippen Method |
| mcvol         | 93.170  | ml/mol | McGowan Method |
| rinpol        | 1033.00 |        | NIST Webbook   |
| rinpol        | 1033.00 |        | NIST Webbook   |

## Sources

|                                                                            |                                                                                                                                           |
|----------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method:                                                            | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| Solubility of Pyrazine and Its Derivatives in Supercritical Carbon Dioxide | <a href="https://www.doi.org/10.1021/je0601457">https://www.doi.org/10.1021/je0601457</a>                                                 |
| 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=U109047&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U109047&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>                                 |

## Legend

|          |                                     |
|----------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l  |
| logp:    | Octanol/Water partition coefficient |
| mcvol:   | McGowan's characteristic volume     |
| rinpol:  | Non-polar retention indices         |

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