

# Pyrazine, 2-methyl-3-(2-propenyl)-

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | 2-Allyl-3-methylpyrazine                                   |
| <b>Inchi:</b>               | InChI=1S/C8H10N2/c1-3-4-8-7(2)9-5-6-10-8/h3,5-6H,1,4H2,2H3 |
| <b>InchiKey:</b>            | AQCVFCFCPBWGSY-UHFFFAOYSA-N                                |
| <b>Formula:</b>             | C8H10N2  |
| <b>SMILES:</b>              | C=CCc1nccnc1C  |
| <b>Mol. weight [g/mol]:</b> | 134.18   |
| <b>CAS:</b>                 | 55138-62-0   |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -2.55   |        | Crippen Method |
| logp          | 1.514   |        | Crippen Method |
| mcvol         | 115.480 | ml/mol | McGowan Method |
| ripol         | 1739.00 |        | NIST Webbook   |
| ripol         | 1739.00 |        | NIST Webbook   |
| ripol         | 1739.00 |        | NIST Webbook   |

## Sources

|                        |   |
|------------------------|---|
| <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=C55138620&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C55138620&amp;Units=SI</a> |
| <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>                             |

## 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>ripol:</b>   | Polar retention indices             |

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