

Pyrazine, 2-ethenyl-6-methyl-

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| Other names: | Pyrazine, 2-methyl-6-vinyl- 2-Methyl-6-vinylpyrazine 2-Vinyl-6-methylpyrazine 2-ethenyl-6-methyl pyrazine 6-methyl-2-vinylpyrazine 2-Ethyl-6-vinylpyrazine |
| Inchi: | InChI=1S/C7H8N2/c1-3-7-5-8-4-6(2)9-7/h3-5H,1H2,2H3 |
| InchiKey: | KZXOOWGVLDHDT-UHFFFAOYSA-N |
| Formula: | C7H8N2 |
| SMILES: | C=Cc1cncc(C)n1 |
| Mol. weight [g/mol]: | 120.15 |
| CAS: | 13925-09-2 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -2.30 | | Crippen Method |
| logp | 1.428 | | Crippen Method |
| mcpol | 101.390 | ml/mol | McGowan Method |
| rinpol | 1000.00 | | NIST Webbook |
| rinpol | 1008.00 | | NIST Webbook |
| rinpol | 985.00 | | NIST Webbook |
| rinpol | 1019.00 | | NIST Webbook |
| rinpol | 1002.00 | | NIST Webbook |
| rinpol | 1020.00 | | NIST Webbook |
| rinpol | 1030.00 | | NIST Webbook |
| rinpol | 1017.00 | | NIST Webbook |
| rinpol | 986.00 | | NIST Webbook |
| rinpol | 998.00 | | NIST Webbook |
| rinpol | 1032.00 | | NIST Webbook |
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| rinpol | 1016.00 | | NIST Webbook |
| rinpol | 1043.00 | | NIST Webbook |

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| ripol | 1037.00 | NIST Webbook |
| ripol | 1034.00 | NIST Webbook |
| ripol | 988.00 | NIST Webbook |
| ripol | 1047.00 | NIST Webbook |
| ripol | 996.00 | NIST Webbook |
| ripol | 1032.00 | NIST Webbook |
| ripol | 1035.00 | NIST Webbook |
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| ripol | 1488.00 | NIST Webbook |

Sources

| | |
|------------------------|---|
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C13925092&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
ripol: Polar retention indices

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