# Pyrazine, 2-methyl-6-(1-propenyl)-, (E)-

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|---|---|
| **Other names:** | Pyrazine, 2-methyl-6-propenyl-, (E)- |
| | 2-Methyl-6-[(1E)-1-propenyl]pyrazine |
| | 2-Methyl-6-(1-propenyl) pyrazine, trans |
| | (E)-2-Methyl-6-(1-propenyl)pyrazine |
| | 2-Methyl-6-(trans-1-propenyl)pyrazine |
| | 2-Methyl-6-[(E)-1-propenyl]pyrazine |
| **Inchi:** | InChI=1S/C8H10N2/c1-3-4-8-6-9-5-7(2)10-8/h3-6H,1-2H3/b4-3+ |
| **InchiKey:** | NOBVHXZAVPKZQU-ONEGZZNKSA-N |
| **Formula:** | C8H10N2 |
| **SMILES:** | CC=Cc1cncc(C)n1 |
| **Mol. weight [g/mol]:** | 134.18 |
| **CAS:** | 18217-81-7 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -2.72 | | Crippen Method |
| logp | 1.818 | | Crippen Method |
| mcvol | 115.480 | ml/mol | McGowan Method |
| rinpol | 1107.00 | | NIST Webbook |
| rinpol | 1107.00 | | NIST Webbook |
| ripol | 1671.00 | | NIST Webbook |
| ripol | 1671.00 | | NIST Webbook |
| ripol | 1671.00 | | NIST Webbook |

# Sources

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C18217817&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# Legend

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|---|---|
| **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 |