# Pyrazine, 3,5-dimethyl-2-propyl-

| | |
|---|---|
| **Other names:** | 2,6-Dimethyl-3-propylpyrazine |
| | Pyrazine, 2,6-dimethyl-3-propyl- |
| | 3,5-Dimethyl-2-propylpyrazine |
| | 2,6-Dimethyl-3-pyropylpyrazine |
| **Inchi:** | InChI=1S/C9H14N2/c1-4-5-9-8(3)11-7(2)6-10-9/h6H,4-5H2,1-3H3 |
| **InchiKey:** | UTRAUCDSVCDVIW-UHFFFAOYSA-N |
| **Formula:** | C9H14N2 |
| **SMILES:** | CCCc1ncc(C)nc1C |
| **Mol. weight [g/mol]:** | 150.22 |
| **CAS:** | 32350-16-6 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -3.18 | | Crippen Method |
| logp | 2.046 | | Crippen Method |
| mcvol | 133.870 | ml/mol | McGowan Method |
| rinpol | 1131.00 | | NIST Webbook |
| rinpol | 1131.00 | | NIST Webbook |
| rinpol | 1130.00 | | NIST Webbook |
| rinpol | 1151.00 | | NIST Webbook |
| rinpol | 1152.00 | | NIST Webbook |
| rinpol | 1151.00 | | NIST Webbook |
| ripol | 1493.00 | | 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=C32350166&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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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https://www.chemeo.com/cid/31-701-8/Pyrazine-3-5-dimethyl-2-propyl.pdf

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