

# 2,3,5-Trimethyl-6-isopentylpyrazine

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | 2-Isopentyl-3,5,6-trimethylpyrazine<br>2,3,5-trimethyl-6-(3-methylbutyl)pyrazine<br>Pyrazine, 2,3,5-trimethyl-6-(3-methylbutyl)<br>Pyrazine, trimethylisopentyl<br>Trimethylisopentylpyrazine<br>Pyrazine, trimethyl(3-methylbutyl)- |
| <b>Inchi:</b>               | InChI=1S/C12H20N2/c1-8(2)6-7-12-11(5)13-9(3)10(4)14-12/h8H,6-7H2,1-5H3   |
| <b>InchiKey:</b>            | KYVXEZPQRULTLX-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C12H20N2   |
| <b>SMILES:</b>              | <chem>Cc1nc(C)c(CCC(C)C)nc1C</chem>  |
| <b>Mol. weight [g/mol]:</b> | 192.30   |
| <b>CAS:</b>                 | 10132-43-1   |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -4.25   |        | Crippen Method |
| logp          | 2.990   |        | Crippen Method |
| mcvol         | 176.140 | ml/mol | McGowan Method |
| rinpol        | 1381.00 |        | NIST Webbook   |
| rinpol        | 1365.00 |        | NIST Webbook   |
| rinpol        | 1361.00 |        | NIST Webbook   |
| rinpol        | 1379.00 |        | NIST Webbook   |
| rinpol        | 1381.00 |        | NIST Webbook   |
| rinpol        | 1390.00 |        | NIST Webbook   |
| rinpol        | 1406.00 |        | NIST Webbook   |

## Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                             |
| <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=C10132431&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C10132431&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>                                     |

# 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>rinpol:</b>  | Non-polar retention indices         |

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