

# 2-methyl-5-(2-methylbutyl)-3-octylpyrazine

**Other names:** Pyrazine, 2-methyl-5-(2-methylbutyl)-3-octyl  
**Inchi:** InChI=1S/C18H32N2/c1-5-7-8-9-10-11-12-18-16(4)19-14-17(20-18)13-15(3)6-2/h14-15H  
**InchiKey:** MFZVESAUFTENP-UHFFFAOYSA-N  
**Formula:** C18H32N2  
**SMILES:** CCCCCCCc1nc(CC(C)CC)cnc1C  
**Mol. weight [g/mol]:** 276.46

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -6.61   |        | Crippen Method |
| logp          | 5.277   |        | Crippen Method |
| mcvol         | 260.680 | ml/mol | McGowan Method |
| rinpol        | 1923.00 |        | NIST Webbook   |
| rinpol        | 1923.00 |        | NIST Webbook   |
| ripol         | 2200.00 |        | NIST Webbook   |
| ripol         | 2200.00 |        | NIST Webbook   |

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R38434&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## 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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