

# 2-methoxy-3-butyl pyrazine

|                      |                                                                   |
|----------------------|-------------------------------------------------------------------|
| Other names:         | Pyrazine, 2-butyl-3-methoxy<br>Pyrazine, 3-butyl-2-methoxy        |
| Inchi:               | InChI=1S/C9H14N2O/c1-3-4-5-8-9(12-2)11-7-6-10-8/h6-7H,3-5H2,1-2H3 |
| InchiKey:            | CPYHBHYOFYVTEV-UHFFFAOYSA-N                                       |
| Formula:             | C9H14N2O                                                          |
| SMILES:              | CCCCc1nccnc1OC                                                    |
| Mol. weight [g/mol]: | 166.22                                                            |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -2.76   |        | Crippen Method |
| logp          | 1.828   |        | Crippen Method |
| mcvol         | 139.740 | ml/mol | McGowan Method |
| rinpol        | 1219.00 |        | NIST Webbook   |
| rinpol        | 1219.00 |        | NIST Webbook   |
| ripol         | 1575.00 |        | NIST Webbook   |
| ripol         | 1575.00 |        | NIST Webbook   |

## Sources

|                 |                                                                                                                                         |
|-----------------|-----------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                               |
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                       |
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                   |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R43613&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R43613&amp;Units=SI</a> |

## 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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