

# Benzamide, 3,4-dimethoxy-N-methyl-

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C10H13NO3/c1-11-10(12)7-4-5-8(13-2)9(6-7)14-3/h4-6H,1-3H3,(H,11,12) |
| <b>InchiKey:</b>            | GFQRPMWTUUBTN-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C10H13NO3  |
| <b>SMILES:</b>              | CN=C(O)c1ccc(OC)c(OC)c1  |
| <b>Mol. weight [g/mol]:</b> | 195.22   |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| hf            | -380.38 | kJ/mol | Joback Method  |
| hvap          | 66.35   | kJ/mol | Joback Method  |
| log10ws       | -1.60   |        | Crippen Method |
| logp          | 1.638   |        | Crippen Method |
| mcvol         | 151.290 | ml/mol | McGowan Method |
| pc            | 2715.50 | kPa    | Joback Method  |
| rinpol        | 1918.00 |        | NIST Webbook   |
| rinpol        | 1918.00 |        | NIST Webbook   |
| tb            | 678.42  | K      | Joback Method  |
| tc            | 886.92  | K      | Joback Method  |

## Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U407998&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U407998&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |

## Legend

|              |   |
|--------------|---|
| <b>hf:</b>   | Enthalpy of formation at standard conditions    |
| <b>hvap:</b> | Enthalpy of vaporization at standard conditions |

|                 |                                     |
|-----------------|-------------------------------------|
| <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>pc:</b>      | Critical Pressure                   |
| <b>rinpol:</b>  | Non-polar retention indices         |
| <b>tb:</b>      | Normal Boiling Point Temperature    |
| <b>tc:</b>      | Critical Temperature                |

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