

# O-Methyl-DL-serine, N-dimethylaminomethylene-, butyl ester

|                      |  |
|----------------------|--|
| Inchi:               | InChI=1S/C11H22N2O3/c1-5-6-7-16-11(14)10(8-15-4)12-9-13(2)3/h9-10H,5-8H2,1-4H3 |
| InchiKey:            | DLLMAHZEJYGNDW-UHFFFAOYSA-N  |
| Formula:             | C11H22N2O3   |
| SMILES:              | CCCCOC(=O)C(COC)N=CN(C)C   |
| Mol. weight [g/mol]: | 230.30   |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| hf            | -502.92 | kJ/mol | Joback Method  |
| hvap          | 56.62   | kJ/mol | Joback Method  |
| log10ws       | -0.72   |        | Crippen Method |
| logp          | 0.935   |        | Crippen Method |
| mcvol         | 194.820 | ml/mol | McGowan Method |
| pc            | 1820.06 | kPa    | Joback Method  |
| rinpol        | 1588.00 |        | NIST Webbook   |
| rinpol        | 1588.00 |        | NIST Webbook   |
| tb            | 638.47  | K      | Joback Method  |
| tc            | 825.03  | K      | Joback Method  |

## Sources

|                 |   |
|-----------------|---|
| Joback Method:  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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=U375995&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U375995&amp;Units=SI</a> |
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>                                 |
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |

## Legend

|       |   |
|-------|---|
| hf:   | Enthalpy of formation at standard conditions    |
| hvap: | 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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