# O-Benzyl-L-serine, N-dimethylaminomethylene-, ethyl ester

**Inchi:** InChI=1S/C15H22N2O3/c1-4-20-15(18)14(16-12-17(2)3)11-19-10-13-8-6-5-7-9-13/h5-9,1

**InchiKey:** ZMJYEGXYBLHNQT-UHFFFAOYSA-N

**Formula:** C15H22N2O3

**SMILES:** CCOC(=O)C(COCc1ccccc1)N=CN(C)C

**Mol. weight [g/mol]:** 278.35

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -348.95 | kJ/mol | Joback Method |
| hvap | 67.80 | kJ/mol | Joback Method |
| log10ws | -1.99 | | Crippen Method |
| logp | 1.725 | | Crippen Method |
| mcvol | 227.420 | ml/mol | McGowan Method |
| pc | 1740.46 | kPa | Joback Method |
| rinpol | 2033.00 | | NIST Webbook |
| rinpol | 2033.00 | | NIST Webbook |
| tb | 756.67 | K | Joback Method |
| tc | 966.84 | K | Joback Method |

## Sources

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

**Joback Method:** https://en.wikipedia.org/wiki/Joback_method

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=U375825&Units=SI

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

## Legend

**hf:** Enthalpy of formation at standard conditions

**hvap:** Enthalpy of vaporization at standard conditions

| | |
|---|---|
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |