

# Tybamate

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | Carbamic acid, butyl-, 2-[[[(aminocarbonyl)oxy]methyl]-2-methylpentyl ester<br>Carbamic acid, butyl-, 2-(hydroxymethyl)-2-methylpentyl ester carbamate (ester)<br>Benvil<br>Depran<br>Effisax<br>Nospan<br>Reposan<br>Solacen<br>Solacin<br>Tibamate<br>Tibamax<br>Tybatran<br>W 713<br>2-Methyl-2-Propyltrimethylene butylcarbamate carbamate<br>n-Butyl-2-methyl-2-propyl-1,3-propanediol dicarbamate<br>Carbamic acid, butyl-, ester with 2-(hydroxymethyl)-2-methylpentyl carbamate<br>Carbamic acid, butyl-, 2-(hydroxymethyl)-2-methylpentyl ester carbamate<br>Carbamic acid, ester with 2-(hydroxymethyl)-2-methylpentyl butylcarbamate<br>Carbamic acid, ester with 2-methyl-2-propyl-1,3-propanediol butylcarbamate<br>Idalene<br>Tibamato<br>1,3-Propanediol, 2-methyl-2-propyl-, butylcarbamate carbamate<br>2-(Hydroxymethyl)-2-(methylpentyl) butylcarbamate carbamate<br>2-Methyl-2-propyl-1,3-propanediol butylcarbamate carbamate<br>N-n-Butyl-2-methyl-2-propyl-1,3-propanediol dicarbamate<br>NSC 172126<br>Carbamic acid, butyl-, 3-hydroxy-2-methyl-2-propyl carbamate ester<br>1,3-Propanediol, 2-methyl-2-propyl-n-butyl dicarbamate |
| <b>Inchi:</b>               | InChI=1S/C13H26N2O4/c1-4-6-8-15-12(17)19-10-13(3,7-5-2)9-18-11(14)16/h4-10H2,1-3  |
| <b>InchiKey:</b>            | PRBORDFJHHAISJ-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C13H26N2O4  |
| <b>SMILES:</b>              | CCCCNC(=O)OCC(C)(CCC)COC(N)=O   |
| <b>Mol. weight [g/mol]:</b> | 274.36  |
| <b>CAS:</b>                 | 4268-36-4   |

## Physical Properties

| Property code | Value | Unit | Source |
|---------------|-------|------|--------|
|---------------|-------|------|--------|

|         |         |  |                      |                |
|---------|---------|--|----------------------|----------------|
| gf      | -250.58 |  | kJ/mol               | Joback Method  |
| hf      | -722.74 |  | kJ/mol               | Joback Method  |
| hfus    | 37.88   |  | kJ/mol               | Joback Method  |
| hvap    | 78.62   |  | kJ/mol               | Joback Method  |
| log10ws | -3.33   |  |                      | Crippen Method |
| logp    | 2.414   |  |                      | Crippen Method |
| mcvol   | 228.870 |  | ml/mol               | McGowan Method |
| pc      | 1915.26 |  | kPa                  | Joback Method  |
| tb      | 768.89  |  | K                    | Joback Method  |
| tc      | 963.74  |  | K                    | Joback Method  |
| tf      | 518.93  |  | K                    | Joback Method  |
| vc      | 0.865   |  | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 695.83 | J/mol×K | 768.89          | Joback Method |
| cpg           | 710.20 | J/mol×K | 801.37          | Joback Method |
| cpg           | 723.67 | J/mol×K | 833.84          | Joback Method |
| cpg           | 736.26 | J/mol×K | 866.32          | Joback Method |
| cpg           | 748.00 | J/mol×K | 898.79          | Joback Method |
| cpg           | 758.92 | J/mol×K | 931.27          | Joback Method |
| cpg           | 769.02 | J/mol×K | 963.74          | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>                       |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C4268364&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4268364&amp;Units=SI</a> |

## Legend

**cpg:** Ideal gas heat capacity

|                 |   |
|-----------------|---|
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion 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>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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