

# Verbenyl propyl ether

|                      |                                                                                  |
|----------------------|----------------------------------------------------------------------------------|
| Other names:         | Verbenol propyl ether                                                            |
| Inchi:               | InChI=1S/C13H22O/c1-5-6-14-12-7-9(2)10-8-11(12)13(10,3)4/h7,10-12H,5-6,8H2,1-4H3 |
| InchiKey:            | GREQYBWLTCPCAU-UHFFFAOYSA-N                                                      |
| Formula:             | C13H22O                                                                          |
| SMILES:              | CCCOC1C=C(C)C2CC1C2(C)C                                                          |
| Mol. weight [g/mol]: | 194.31                                                                           |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 62.40   | kJ/mol  | Joback Method  |
| hf            | -283.56 | kJ/mol  | Joback Method  |
| hfus          | 21.46   | kJ/mol  | Joback Method  |
| hvap          | 46.12   | kJ/mol  | Joback Method  |
| log10ws       | -3.38   |         | Crippen Method |
| logp          | 3.404   |         | Crippen Method |
| mcvol         | 173.880 | ml/mol  | McGowan Method |
| pc            | 2069.88 | kPa     | Joback Method  |
| rinpol        | 1302.00 |         | NIST Webbook   |
| tb            | 532.05  | K       | Joback Method  |
| tc            | 730.96  | K       | Joback Method  |
| tf            | 319.56  | K       | Joback Method  |
| vc            | 0.669   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 443.22 | J/mol×K | 532.05          | Joback Method |
| cpg           | 462.70 | J/mol×K | 565.20          | Joback Method |
| cpg           | 481.09 | J/mol×K | 598.35          | Joback Method |
| cpg           | 498.48 | J/mol×K | 631.50          | Joback Method |
| cpg           | 515.00 | J/mol×K | 664.65          | Joback Method |
| cpg           | 530.73 | J/mol×K | 697.80          | Joback Method |
| cpg           | 545.79 | J/mol×K | 730.96          | Joback Method |

# Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U108772&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U108772&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>cpg:</b>     | 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>rlnpol:</b>  | Non-polar retention indices                     |
| <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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