

# 1,10-Di-epcubenol

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C15H26O/c1-10(2)13-6-5-12(4)15(16)8-7-11(3)9-14(13)15/h9-10,12-14,16H,5- |
| <b>InchiKey:</b>            | COGPRPSWSKLTQF-XQLPTFJDSA-N   |
| <b>Formula:</b>             | C15H26O   |
| <b>SMILES:</b>              | CC1=CC2C(C(C)C)CCC(C)C2(O)CC1   |
| <b>Mol. weight [g/mol]:</b> | 222.37  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 8.68    | kJ/mol               | Joback Method  |
| hf            | -368.61 | kJ/mol               | Joback Method  |
| hfus          | 19.72   | kJ/mol               | Joback Method  |
| hvap          | 64.97   | kJ/mol               | Joback Method  |
| log10ws       | -4.15   |                      | Crippen Method |
| logp          | 3.776   |                      | Crippen Method |
| mcvol         | 202.060 | ml/mol               | McGowan Method |
| pc            | 2069.88 | kPa                  | Joback Method  |
| rinpol        | 1598.00 |                      | NIST Webbook   |
| tb            | 659.94  | K                    | Joback Method  |
| tc            | 865.11  | K                    | Joback Method  |
| tf            | 355.13  | K                    | Joback Method  |
| vc            | 0.752   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 597.80 | J/mol×K | 659.94          | Joback Method |
| cpg           | 617.79 | J/mol×K | 694.13          | Joback Method |
| cpg           | 636.77 | J/mol×K | 728.33          | Joback Method |
| cpg           | 654.86 | J/mol×K | 762.52          | Joback Method |
| cpg           | 672.18 | J/mol×K | 796.72          | Joback Method |
| cpg           | 688.83 | J/mol×K | 830.91          | Joback Method |
| cpg           | 704.93 | J/mol×K | 865.11          | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <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=R334344&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R334344&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>                                     |

# 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>rinpola:</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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