

# Longipinocarveol, trans-

|                      |                                                                                   |
|----------------------|-----------------------------------------------------------------------------------|
| Other names:         | trans-Longipinocarveol                                                            |
| Inchi:               | InChI=1S/C15H24O/c1-10-12(16)8-11-9-15(10)13(2,3)6-5-7-14(11,15)4/h11-12,16H,1,5- |
| InchiKey:            | QZIBYWPRLPFUFP-UHFFFAOYSA-N                                                       |
| Formula:             | C15H24O                                                                           |
| SMILES:              | C=C1C(O)CC2CC13C(C)(C)CCCC23C                                                     |
| Mol. weight [g/mol]: | 220.35                                                                            |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 117.84  | kJ/mol  | Joback Method  |
| hf            | -209.80 | kJ/mol  | Joback Method  |
| hfus          | 10.99   | kJ/mol  | Joback Method  |
| hvap          | 61.83   | kJ/mol  | Joback Method  |
| log10ws       | -4.05   |         | Crippen Method |
| logp          | 3.530   |         | Crippen Method |
| mcvol         | 191.200 | ml/mol  | McGowan Method |
| pc            | 2407.64 | kPa     | Joback Method  |
| rinpol        | 1618.00 |         | NIST Webbook   |
| tb            | 654.08  | K       | Joback Method  |
| tc            | 869.16  | K       | Joback Method  |
| tf            | 443.31  | K       | Joback Method  |
| vc            | 0.726   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 570.34 | J/mol×K | 654.08          | Joback Method |
| cpg           | 588.87 | J/mol×K | 689.93          | Joback Method |
| cpg           | 606.74 | J/mol×K | 725.77          | Joback Method |
| cpg           | 624.31 | J/mol×K | 761.62          | Joback Method |
| cpg           | 641.90 | J/mol×K | 797.47          | Joback Method |
| cpg           | 659.86 | J/mol×K | 833.31          | Joback Method |
| cpg           | 678.52 | J/mol×K | 869.16          | Joback Method |

# Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <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=U159365&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U159365&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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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