

# 9,10-dehydroisolongifolene

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C15H22/c1-13(2)8-5-6-12-14(3,4)11-7-9-15(12,13)10-11/h5-6,8,11H,7,9-10H2, |
| <b>InchiKey:</b>            | UIPKEVNEOFKIRG-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C15H22   |
| <b>SMILES:</b>              | CC1(C)C2=CC=CC(C)(C)C23CCC1C3  |
| <b>Mol. weight [g/mol]:</b> | 202.34   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 259.58  | kJ/mol               | Joback Method  |
| hf            | -17.38  | kJ/mol               | Joback Method  |
| hfus          | 9.04    | kJ/mol               | Joback Method  |
| hvap          | 46.55   | kJ/mol               | Joback Method  |
| log10ws       | -4.53   |                      | Crippen Method |
| logp          | 4.335   |                      | Crippen Method |
| mcvol         | 181.030 | ml/mol               | McGowan Method |
| pc            | 2358.78 | kPa                  | Joback Method  |
| rinpol        | 1558.00 |                      | NIST Webbook   |
| rinpol        | 1508.00 |                      | NIST Webbook   |
| tb            | 570.71  | K                    | Joback Method  |
| tc            | 808.01  | K                    | Joback Method  |
| tf            | 387.09  | K                    | Joback Method  |
| vc            | 0.696   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 481.77 | J/mol×K | 570.71          | Joback Method |
| cpg           | 502.91 | J/mol×K | 610.26          | Joback Method |
| cpg           | 522.45 | J/mol×K | 649.81          | Joback Method |
| cpg           | 540.85 | J/mol×K | 689.36          | Joback Method |
| cpg           | 558.58 | J/mol×K | 728.91          | Joback Method |
| cpg           | 576.10 | J/mol×K | 768.46          | Joback Method |
| cpg           | 593.88 | J/mol×K | 808.01          | 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=R322084&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R322084&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>                         |
| <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>hvp:</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>rinp:</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                                 |

Latest version available from:

<https://www.cheméo.com/cid/28-976-8/9-10-dehydroisolongifolene.pdf>

Generated by Cheméo on 2024-04-27 23:21:45.302449864 +0000 UTC m=+16549354.223027175.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.