

# Cyclohexanol,5-(1,1-dimethylethyl)-2-methylene-t

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C11H20O/c1-8-5-6-9(7-10(8)12)11(2,3)4/h9-10,12H,1,5-7H2,2-4H3/t9-,10+/m0 |
| <b>InchiKey:</b>            | MKWJZCGGUSWUQL-VHSXEESVSA-N   |
| <b>Formula:</b>             | C11H20O   |
| <b>SMILES:</b>              | C=C1CCC(C(C)(C)C)CC1O   |
| <b>Mol. weight [g/mol]:</b> | 168.28  |
| <b>CAS:</b>                 | 19245-70-6  |

## Physical Properties

| Property code | Value       | Unit    | Source         |
|---------------|-------------|---------|----------------|
| gf            | -22.42      | kJ/mol  | Joback Method  |
| hf            | -313.13     | kJ/mol  | Joback Method  |
| hfus          | 12.67       | kJ/mol  | Joback Method  |
| hvap          | 55.74       | kJ/mol  | Joback Method  |
| ie            | 9.37 ± 0.02 | eV      | NIST Webbook   |
| ie            | 9.37 ± 0.05 | eV      | NIST Webbook   |
| log10ws       | -3.07       |         | Crippen Method |
| logp          | 2.750       |         | Crippen Method |
| mcvol         | 156.560     | ml/mol  | McGowan Method |
| pc            | 2571.50     | kPa     | Joback Method  |
| tb            | 554.07      | K       | Joback Method  |
| tc            | 750.02      | K       | Joback Method  |
| tf            | 293.79      | K       | Joback Method  |
| vc            | 0.576       | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 402.06 | J/molxK | 554.07          | Joback Method |
| cpg           | 479.03 | J/molxK | 717.36          | Joback Method |
| cpg           | 465.38 | J/molxK | 684.70          | Joback Method |
| cpg           | 450.89 | J/molxK | 652.04          | Joback Method |
| cpg           | 435.53 | J/molxK | 619.39          | Joback Method |
| cpg           | 419.26 | J/molxK | 586.73          | Joback Method |
| cpg           | 491.87 | J/molxK | 750.02          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0001194 | Paxs | 554.07 | Joback Method |
| dvisc | 0.0001900 | Paxs | 510.69 | Joback Method |
| dvisc | 0.0003297 | Paxs | 467.31 | Joback Method |
| dvisc | 0.0006401 | Paxs | 423.93 | Joback Method |
| dvisc | 0.0014460 | Paxs | 380.55 | Joback Method |
| dvisc | 0.0040285 | Paxs | 337.17 | Joback Method |
| dvisc | 0.0151885 | Paxs | 293.79 | 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=C19245706&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C19245706&amp;Units=SI</a> |

## Legend

|                 |   |
|-----------------|---|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>dvisc:</b>   | Dynamic viscosity                               |
| <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>ie:</b>      | Ionization energy                               |
| <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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