

# 1,1,2,4-tetramethylcyclohexane, trans, cis

|                      |                                                                        |
|----------------------|------------------------------------------------------------------------|
| Other names:         | Cyclohexane, 1,1,2,4-tetramethyl, cis                                  |
| Inchi:               | InChI=1S/C10H20/c1-8-5-6-10(3,4)9(2)7-8/h8-9H,5-7H2,1-4H3/t8-,9+/m0/s1 |
| InchiKey:            | YPLGUQUVOXNUBM-DTWKUNHWSA-N                                            |
| Formula:             | C10H20                                                                 |
| SMILES:              | CC1CCC(C)(C)C(C)C1                                                     |
| Mol. weight [g/mol]: | 140.27                                                                 |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 36.86   | kJ/mol  | Joback Method  |
| hf            | -220.85 | kJ/mol  | Joback Method  |
| hfus          | 9.33    | kJ/mol  | Joback Method  |
| hvap          | 36.51   | kJ/mol  | Joback Method  |
| log10ws       | -3.18   |         | Crippen Method |
| logp          | 3.469   |         | Crippen Method |
| mcvol         | 140.900 | ml/mol  | McGowan Method |
| pc            | 2515.07 | kPa     | Joback Method  |
| rinpol        | 816.50  |         | NIST Webbook   |
| tb            | 438.65  | K       | Joback Method  |
| tc            | 643.42  | K       | Joback Method  |
| tf            | 225.26  | K       | Joback Method  |
| vc            | 0.524   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 300.31 | J/mol×K | 438.65          | Joback Method |
| cpg           | 321.00 | J/mol×K | 472.78          | Joback Method |
| cpg           | 340.50 | J/mol×K | 506.91          | Joback Method |
| cpg           | 358.88 | J/mol×K | 541.03          | Joback Method |
| cpg           | 376.24 | J/mol×K | 575.16          | Joback Method |
| cpg           | 392.65 | J/mol×K | 609.29          | Joback Method |
| cpg           | 408.21 | J/mol×K | 643.42          | Joback Method |

# Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R141098&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R141098&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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