

# Cyclohexane, 1,4-dimethyl-

|                      |                                                                                                                                                                                    |
|----------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | p-Dimethylcyclohexane<br>1,4-Dimethylcyclohexane<br>1,4-Dimethylcyclohexane,c&t<br>cis-trans-1,4-Dimethylcyclohexane<br>Hexahydroxylene<br>UN 2263<br>1,4-Dimethylcyclohexane(c,t) |
| Inchi:               | InChI=1S/C8H16/c1-7-3-5-8(2)6-4-7/h7-8H,3-6H2,1-2H3                                                                                                                                |
| InchiKey:            | QRMPKOFEUHIBNM-UHFFFAOYSA-N                                                                                                                                                        |
| Formula:             | C8H16                                                                                                                                                                              |
| SMILES:              | CC1CCC(C)CC1                                                                                                                                                                       |
| Mol. weight [g/mol]: | 112.21                                                                                                                                                                             |
| CAS:                 | 589-90-2                                                                                                                                                                           |

## Physical Properties

| Property code | Value    | Unit   | Source         |
|---------------|----------|--------|----------------|
| chl           | -5183.10 | kJ/mol | NIST Webbook   |
| gf            | 33.22    | kJ/mol | Joback Method  |
| hf            | -174.47  | kJ/mol | Joback Method  |
| hfus          | 9.38     | kJ/mol | Joback Method  |
| hvap          | 33.52    | kJ/mol | Joback Method  |
| log10ws       | -2.58    |        | Crippen Method |
| logp          | 2.833    |        | Crippen Method |
| mcvol         | 112.720  | ml/mol | McGowan Method |
| pc            | 3038.96  | kPa    | Joback Method  |
| rinpol        | 807.00   |        | NIST Webbook   |
| rinpol        | 821.00   |        | NIST Webbook   |
| rinpol        | 782.00   |        | NIST Webbook   |
| rinpol        | 777.00   |        | NIST Webbook   |
| rinpol        | 805.00   |        | NIST Webbook   |
| rinpol        | 811.42   |        | NIST Webbook   |
| rinpol        | 805.00   |        | NIST Webbook   |
| rinpol        | 806.30   |        | NIST Webbook   |
| rinpol        | 814.00   |        | NIST Webbook   |
| rinpol        | 803.00   |        | NIST Webbook   |
| rinpol        | 771.00   |        | NIST Webbook   |
| rinpol        | 785.00   |        | NIST Webbook   |

|        |               |         |               |
|--------|---------------|---------|---------------|
| rinpol | 789.00        |         | NIST Webbook  |
| rinpol | 785.00        |         | NIST Webbook  |
| rinpol | 810.00        |         | NIST Webbook  |
| rinpol | 801.00        |         | NIST Webbook  |
| rinpol | 805.00        |         | NIST Webbook  |
| tb     | 410.65 ± 3.00 | K       | NIST Webbook  |
| tb     | 393.20        | K       | NIST Webbook  |
| tb     | 393.00 ± 2.00 | K       | NIST Webbook  |
| tb     | 392.00 ± 2.00 | K       | NIST Webbook  |
| tb     | 396.00 ± 1.00 | K       | NIST Webbook  |
| tb     | 393.30 ± 1.00 | K       | NIST Webbook  |
| tb     | 396.20 ± 3.00 | K       | NIST Webbook  |
| tb     | 397.74 ± 0.40 | K       | NIST Webbook  |
| tb     | 393.80 ± 0.50 | K       | NIST Webbook  |
| tb     | 394.90 ± 1.50 | K       | NIST Webbook  |
| tb     | 396.30 ± 1.00 | K       | NIST Webbook  |
| tb     | 392.90 ± 2.00 | K       | NIST Webbook  |
| tc     | 597.67        | K       | Joback Method |
| tf     | 183.06        | K       | Joback Method |
| vc     | 0.415         | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 212.54    | J/mol×K | 397.32          | Joback Method |
| cpg           | 230.28    | J/mol×K | 430.71          | Joback Method |
| cpg           | 247.23    | J/mol×K | 464.10          | Joback Method |
| cpg           | 263.41    | J/mol×K | 497.49          | Joback Method |
| cpg           | 278.84    | J/mol×K | 530.89          | Joback Method |
| cpg           | 293.52    | J/mol×K | 564.28          | Joback Method |
| cpg           | 307.47    | J/mol×K | 597.67          | Joback Method |
| dvisc         | 0.0041986 | Pa×s    | 183.06          | Joback Method |
| dvisc         | 0.0018154 | Pa×s    | 218.77          | Joback Method |
| dvisc         | 0.0009932 | Pa×s    | 254.48          | Joback Method |
| dvisc         | 0.0006303 | Pa×s    | 290.19          | Joback Method |
| dvisc         | 0.0004419 | Pa×s    | 325.90          | Joback Method |
| dvisc         | 0.0003324 | Pa×s    | 361.61          | Joback Method |
| dvisc         | 0.0002631 | Pa×s    | 397.32          | Joback Method |

# Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <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>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C589902&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C589902&amp;Units=SI</a> |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>chl:</b>     | Standard liquid enthalpy of combustion          |
| <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>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>rinpol:</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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