

# Cyclohexane, 1-(cyclohexylmethyl)-3-methyl-, cis-

|                      |                                                                                   |
|----------------------|-----------------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C14H26/c1-12-6-5-9-14(10-12)11-13-7-3-2-4-8-13/h12-14H,2-11H2,1H3/t12-,1 |
| InchiKey:            | XJVUTISPBKZNB-GXTWGEPZSA-N                                                        |
| Formula:             | C14H26                                                                            |
| SMILES:              | CC1CCCC(CC2CCCCC2)C1                                                              |
| Mol. weight [g/mol]: | 194.36                                                                            |
| CAS:                 | 54823-96-0                                                                        |

## Physical Properties

| Property code | Value    | Unit    | Source         |
|---------------|----------|---------|----------------|
| chl           | -8305.00 | kJ/mol  | NIST Webbook   |
| gf            | 108.19   | kJ/mol  | Joback Method  |
| hf            | -243.99  | kJ/mol  | Joback Method  |
| hfus          | 16.76    | kJ/mol  | Joback Method  |
| hvap          | 47.31    | kJ/mol  | Joback Method  |
| log10ws       | -4.75    |         | Crippen Method |
| logp          | 4.783    |         | Crippen Method |
| mcvol         | 186.400  | ml/mol  | McGowan Method |
| pc            | 2094.58  | kPa     | Joback Method  |
| tb            | 554.15   | K       | Joback Method  |
| tc            | 777.71   | K       | Joback Method  |
| tf            | 258.06   | K       | Joback Method  |
| vc            | 0.684    | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 490.28    | J/mol×K | 554.15          | Joback Method |
| cpg           | 610.19    | J/mol×K | 740.45          | Joback Method |
| cpg           | 589.27    | J/mol×K | 703.19          | Joback Method |
| cpg           | 566.87    | J/mol×K | 665.93          | Joback Method |
| cpg           | 542.93    | J/mol×K | 628.67          | Joback Method |
| cpg           | 517.42    | J/mol×K | 591.41          | Joback Method |
| cpg           | 629.67    | J/mol×K | 777.71          | Joback Method |
| dvisc         | 0.0002391 | Pa×s    | 554.15          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0003187 | Pa×s | 504.80 | Joback Method |
| dvisc | 0.0004522 | Pa×s | 455.45 | Joback Method |
| dvisc | 0.0006984 | Pa×s | 406.10 | Joback Method |
| dvisc | 0.0012166 | Pa×s | 356.76 | Joback Method |
| dvisc | 0.0025328 | Pa×s | 307.41 | Joback Method |
| dvisc | 0.0069798 | Pa×s | 258.06 | 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=C54823960&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C54823960&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>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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