

# 1,1'-Bicyclohexyl, 2-(1-methylethyl)-, cis-

|                      |                                                                                   |
|----------------------|-----------------------------------------------------------------------------------|
| Other names:         | Bicyclohexyl, 2-isopropyl-, cis-                                                  |
| Inchi:               | InChI=1S/C15H28/c1-12(2)14-10-6-7-11-15(14)13-8-4-3-5-9-13/h12-15H,3-11H2,1-2H3/t |
| InchiKey:            | XWULVJMSQHXLOJ-LSDHHAIUSA-N                                                       |
| Formula:             | C15H28                                                                            |
| SMILES:              | CC(C)C1CCCCC1C1CCCCC1                                                             |
| Mol. weight [g/mol]: | 208.38                                                                            |
| CAS:                 | 50991-15-6                                                                        |

## Physical Properties

| Property code | Value    | Unit    | Source         |
|---------------|----------|---------|----------------|
| chs           | -8954.00 | kJ/mol  | NIST Webbook   |
| gf            | 114.17   | kJ/mol  | Joback Method  |
| hf            | -269.91  | kJ/mol  | Joback Method  |
| hfus          | 15.82    | kJ/mol  | Joback Method  |
| hvap          | 49.14    | kJ/mol  | Joback Method  |
| log10ws       | -4.92    |         | Crippen Method |
| logp          | 5.029    |         | Crippen Method |
| mcvol         | 200.490  | ml/mol  | McGowan Method |
| pc            | 1935.54  | kPa     | Joback Method  |
| tb            | 576.59   | K       | Joback Method  |
| tc            | 800.93   | K       | Joback Method  |
| tf            | 254.33   | K       | Joback Method  |
| vc            | 0.735    | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 545.45 | J/mol×K | 576.59          | Joback Method |
| cpg           | 573.36 | J/mol×K | 613.98          | Joback Method |
| cpg           | 599.56 | J/mol×K | 651.37          | Joback Method |
| cpg           | 624.09 | J/mol×K | 688.76          | Joback Method |
| cpg           | 647.02 | J/mol×K | 726.15          | Joback Method |
| cpg           | 668.39 | J/mol×K | 763.54          | Joback Method |
| cpg           | 688.24 | J/mol×K | 800.93          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0098872 | Pa×s | 254.33 | Joback Method |
| dvisc | 0.0029553 | Pa×s | 308.04 | Joback Method |
| dvisc | 0.0012644 | Pa×s | 361.75 | Joback Method |
| dvisc | 0.0006737 | Pa×s | 415.46 | Joback Method |
| dvisc | 0.0004147 | Pa×s | 469.17 | Joback Method |
| dvisc | 0.0002820 | Pa×s | 522.88 | Joback Method |
| dvisc | 0.0002060 | Pa×s | 576.59 | 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=C50991156&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C50991156&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>                             |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                         |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>chs:</b>     | Standard solid 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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