

# cis-Bicyclo[4.3.0]-3-nonene

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | 2,3,3a,4,7,7a-Hexahydro-1H-indene                            |
| <b>Inchi:</b>               | InChI=1S/C9H14/c1-2-5-9-7-3-6-8(9)4-1/h1-2,8-9H,3-7H2/t8-,9+ |
| <b>InchiKey:</b>            | UZURTQHPMXADGG-DTORHVGOSA-N                                  |
| <b>Formula:</b>             | C9H14  |
| <b>SMILES:</b>              | C1=CCC2CCCC2C1   |
| <b>Mol. weight [g/mol]:</b> | 122.21   |
| <b>CAS:</b>                 | 85236-78-8   |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 140.06  | kJ/mol  | Joback Method  |
| hf            | -44.19  | kJ/mol  | Joback Method  |
| hfus          | 10.26   | kJ/mol  | Joback Method  |
| hvap          | 36.26   | kJ/mol  | Joback Method  |
| log10ws       | -2.75   |         | Crippen Method |
| logp          | 2.753   |         | Crippen Method |
| mcvol         | 111.650 | ml/mol  | McGowan Method |
| pc            | 3415.86 | kPa     | Joback Method  |
| rinpol        | 1038.00 |         | NIST Webbook   |
| tb            | 430.77  | K       | Joback Method  |
| tc            | 649.36  | K       | Joback Method  |
| tf            | 217.27  | K       | Joback Method  |
| vc            | 0.415   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 226.80 | J/molxK | 430.77          | Joback Method |
| cpg           | 245.93 | J/molxK | 467.20          | Joback Method |
| cpg           | 263.83 | J/molxK | 503.63          | Joback Method |
| cpg           | 280.56 | J/molxK | 540.06          | Joback Method |
| cpg           | 296.19 | J/molxK | 576.50          | Joback Method |
| cpg           | 310.78 | J/molxK | 612.93          | Joback Method |
| cpg           | 324.39 | J/molxK | 649.36          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0020254 | Paxs | 217.27 | Joback Method |
| dvisc | 0.0013118 | Paxs | 252.85 | Joback Method |
| dvisc | 0.0009458 | Paxs | 288.44 | Joback Method |
| dvisc | 0.0007327 | Paxs | 324.02 | Joback Method |
| dvisc | 0.0005970 | Paxs | 359.60 | Joback Method |
| dvisc | 0.0005047 | Paxs | 395.19 | Joback Method |
| dvisc | 0.0004387 | Paxs | 430.77 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <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=C85236788&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C85236788&amp;Units=SI</a> |
| <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>                                     |

## 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>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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