

# 1-methyl-cis-2-(1-trans-propenyl)-cyclopropane

|                      |                                                                        |
|----------------------|------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C7H12/c1-3-4-7-5-6(7)2/h3-4,6-7H,5H2,1-2H3/b4-3+/t6-,7+/m1/s1 |
| InchiKey:            | LNAVSCYUHFMDNS-OHUBKANTSA-N                                            |
| Formula:             | C7H12                                                                  |
| SMILES:              | CC=CC1CC1C                                                             |
| Mol. weight [g/mol]: | 96.17                                                                  |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 141.32  | kJ/mol  | Joback Method  |
| hf            | -18.13  | kJ/mol  | Joback Method  |
| hfus          | 13.29   | kJ/mol  | Joback Method  |
| hvap          | 30.74   | kJ/mol  | Joback Method  |
| log10ws       | -2.02   |         | Crippen Method |
| logp          | 2.219   |         | Crippen Method |
| mcvol         | 94.330  | ml/mol  | McGowan Method |
| pc            | 3299.15 | kPa     | Joback Method  |
| rinpol        | 719.70  |         | NIST Webbook   |
| rinpol        | 720.10  |         | NIST Webbook   |
| rinpol        | 720.40  |         | NIST Webbook   |
| tb            | 365.79  | K       | Joback Method  |
| tc            | 552.98  | K       | Joback Method  |
| tf            | 177.27  | K       | Joback Method  |
| vc            | 0.363   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 163.81 | J/mol×K | 365.79          | Joback Method |
| cpg           | 177.37 | J/mol×K | 396.99          | Joback Method |
| cpg           | 190.19 | J/mol×K | 428.19          | Joback Method |
| cpg           | 202.31 | J/mol×K | 459.38          | Joback Method |
| cpg           | 213.75 | J/mol×K | 490.58          | Joback Method |
| cpg           | 224.57 | J/mol×K | 521.78          | Joback Method |
| cpg           | 234.79 | J/mol×K | 552.98          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0003994 | Pa×s | 177.27 | Joback Method |
| dvisc | 0.0003421 | Pa×s | 208.69 | Joback Method |
| dvisc | 0.0003051 | Pa×s | 240.11 | Joback Method |
| dvisc | 0.0002795 | Pa×s | 271.53 | Joback Method |
| dvisc | 0.0002607 | Pa×s | 302.95 | Joback Method |
| dvisc | 0.0002464 | Pa×s | 334.37 | Joback Method |
| dvisc | 0.0002351 | Pa×s | 365.79 | 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=R137287&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R137287&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>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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