

# 1,3-CYCLOPENTADIENE, 5-(1,1-DIMETHYLETHYL)-

Other names: 5-tert-Butyl-1,3-cyclopentadiene  
Inchi: InChI=1S/C9H14/c1-9(2,3)8-6-4-5-7-8/h4-8H,1-3H3  
InchiKey: ZATNUISQHWOHKK-UHFFFAOYSA-N  
Formula: C9H14  
SMILES: CC(C)(C)C1C=CC=C1  
Mol. weight [g/mol]: 122.21

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| hfus          | 8.03    | kJ/mol | Joback Method  |
| logp          | 2.775   |        | Crippen Method |
| mcvol         | 118.210 | ml/mol | McGowan Method |
| rinpol        | 788.00  |        | NIST Webbook   |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 230.51    | J/mol×K | 415.69          | Joback Method |
| cpg           | 247.38    | J/mol×K | 450.45          | Joback Method |
| cpg           | 263.17    | J/mol×K | 485.22          | Joback Method |
| cpg           | 277.92    | J/mol×K | 519.98          | Joback Method |
| cpg           | 291.71    | J/mol×K | 554.75          | Joback Method |
| cpg           | 304.57    | J/mol×K | 589.51          | Joback Method |
| cpg           | 316.56    | J/mol×K | 624.28          | Joback Method |
| dvisc         | 0.0046178 | Pa×s    | 206.03          | Joback Method |
| dvisc         | 0.0021026 | Pa×s    | 240.97          | Joback Method |
| dvisc         | 0.0011685 | Pa×s    | 275.92          | Joback Method |
| dvisc         | 0.0007411 | Pa×s    | 310.86          | Joback Method |
| dvisc         | 0.0005153 | Pa×s    | 345.80          | Joback Method |
| dvisc         | 0.0003830 | Pa×s    | 380.75          | Joback Method |
| dvisc         | 0.0002993 | Pa×s    | 415.69          | Joback Method |

# Sources

**Cheméo Relay (1.0):**

**Cheméo Relay (1.0, beta):**

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C35059406&Units=SI>

**Joback Method:**

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**McGowan Method:**

<http://link.springer.com/article/10.1007/BF02311772>

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## Legend

|                 |                                           |
|-----------------|-------------------------------------------|
| <b>cpg:</b>     | Ideal gas heat capacity                   |
| <b>dvisc:</b>   | Dynamic viscosity                         |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions |
| <b>logp:</b>    | Octanol/Water partition coefficient       |
| <b>mcvol:</b>   | McGowan's characteristic volume           |
| <b>rinpola:</b> | Non-polar retention indices               |

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