

# cis,cis,cis-Bicyclo[4.4.0]decane, 2,5-dimethyl

|                      |                                                                                     |
|----------------------|-------------------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C12H22/c1-9-7-8-10(2)12-6-4-3-5-11(9)12/h9-12H,3-8H2,1-2H3/t9-,10+,11-,12- |
| InchiKey:            | POHSTLAFRROMOQ-BKUVIOGVSA-N                                                         |
| Formula:             | C12H22                                                                              |
| SMILES:              | CC1CCC(C)C2CCCCC12                                                                  |
| Mol. weight [g/mol]: | 166.30                                                                              |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 107.84  | kJ/mol  | Joback Method  |
| hf            | -210.73 | kJ/mol  | Joback Method  |
| hfus          | 16.85   | kJ/mol  | Joback Method  |
| hvap          | 42.20   | kJ/mol  | Joback Method  |
| log10ws       | -3.67   |         | Crippen Method |
| logp          | 3.859   |         | Crippen Method |
| mcvol         | 158.220 | ml/mol  | McGowan Method |
| pc            | 2320.31 | kPa     | Joback Method  |
| rinpol        | 1286.00 |         | NIST Webbook   |
| ripol         | 1446.00 |         | NIST Webbook   |
| tb            | 495.18  | K       | Joback Method  |
| tc            | 710.00  | K       | Joback Method  |
| tf            | 238.32  | K       | Joback Method  |
| vc            | 0.588   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 382.66    | J/mol×K | 495.18          | Joback Method |
| cpg           | 407.11    | J/mol×K | 530.98          | Joback Method |
| cpg           | 430.21    | J/mol×K | 566.79          | Joback Method |
| cpg           | 451.99    | J/mol×K | 602.59          | Joback Method |
| cpg           | 472.51    | J/mol×K | 638.39          | Joback Method |
| cpg           | 491.81    | J/mol×K | 674.20          | Joback Method |
| cpg           | 509.92    | J/mol×K | 710.00          | Joback Method |
| dvisc         | 0.0022593 | Pa×s    | 238.32          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0013842 | Pa×s | 281.13 | Joback Method |
| dvisc | 0.0009653 | Pa×s | 323.94 | Joback Method |
| dvisc | 0.0007322 | Pa×s | 366.75 | Joback Method |
| dvisc | 0.0005885 | Pa×s | 409.56 | Joback Method |
| dvisc | 0.0004929 | Pa×s | 452.37 | Joback Method |
| dvisc | 0.0004257 | Pa×s | 495.18 | Joback Method |

## Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <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>                                     |
| <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=R530968&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R530968&amp;Units=SI</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>ripol:</b>   | 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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