

# Bicyclo[2.2.1]heptane, 2-cyclopropylidene-1,7,7-trimethyl-

|                      |   |
|----------------------|---|
| Other names:         | 2-Cyclopropylidene-1,7,7-trimethylbicyclo[2.2.1]heptane                 |
| Inchi:               | InChI=1S/C13H20/c1-12(2)10-6-7-13(12,3)11(8-10)9-4-5-9/h10H,4-8H2,1-3H3 |
| InchiKey:            | SOXIHOIHJNQQY-UHFFFAOYSA-N  |
| Formula:             | C13H20  |
| SMILES:              | CC12CCC(CC1=C1CC1)C2(C)C  |
| Mol. weight [g/mol]: | 176.30  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 228.45  | kJ/mol               | Joback Method  |
| hf            | -34.09  | kJ/mol               | Joback Method  |
| hfus          | 9.58    | kJ/mol               | Joback Method  |
| hvap          | 43.76   | kJ/mol               | Joback Method  |
| log10ws       | -4.08   |                      | Crippen Method |
| logp          | 3.923   |                      | Crippen Method |
| mcvol         | 157.150 | ml/mol               | McGowan Method |
| pc            | 2616.41 | kPa                  | Joback Method  |
| rinpol        | 1254.00 |                      | NIST Webbook   |
| rinpol        | 1254.00 |                      | NIST Webbook   |
| tb            | 530.93  | K                    | Joback Method  |
| tc            | 757.90  | K                    | Joback Method  |
| tf            | 360.17  | K                    | Joback Method  |
| vc            | 0.609   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 400.97 | J/mol×K | 530.93          | Joback Method |
| cpg           | 420.89 | J/mol×K | 568.76          | Joback Method |
| cpg           | 439.16 | J/mol×K | 606.59          | Joback Method |
| cpg           | 456.11 | J/mol×K | 644.42          | Joback Method |
| cpg           | 472.03 | J/mol×K | 682.25          | Joback Method |
| cpg           | 487.25 | J/mol×K | 720.07          | Joback Method |
| cpg           | 502.07 | J/mol×K | 757.90          | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <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>                                 |
| <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=U159457&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U159457&amp;Units=SI</a> |

# Legend

|                 |   |
|-----------------|---|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <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>hvp:</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>rinp:</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                                 |

Latest version available from:

<https://www.chemeo.com/cid/74-793-0/Bicyclo-2-2-1-heptane-2-cyclopropylidene-1-7-7-trimethyl.pdf>

Generated by Cheméo on 2024-05-06 22:52:17.597565053 +0000 UTC m=+17325186.518142370.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.