

# 1,7,7-Trimethylbicyclo[2.2.1]hept-5-en-2-one

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C10H14O/c1-9(2)7-4-5-10(9,3)8(11)6-7/h4-5,7H,6H2,1-3H3 |
| <b>InchiKey:</b>            | BQJYIYRCGDNPLN-UHFFFAOYSA-N                                     |
| <b>Formula:</b>             | C10H14O   |
| <b>SMILES:</b>              | CC12C=CC(CC1=O)C2(C)C   |
| <b>Mol. weight [g/mol]:</b> | 150.22  |
| <b>CAS:</b>                 | 22516-10-5  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 31.40   | kJ/mol               | Joback Method  |
| hf            | -180.07 | kJ/mol               | Joback Method  |
| hfus          | 5.03    | kJ/mol               | Joback Method  |
| hvap          | 39.78   | kJ/mol               | Joback Method  |
| log10ws       | -2.21   |                      | Crippen Method |
| logp          | 2.178   |                      | Crippen Method |
| mvol          | 127.310 | ml/mol               | McGowan Method |
| pc            | 3210.04 | kPa                  | Joback Method  |
| rinpol        | 1101.90 |                      | NIST Webbook   |
| tb            | 508.74  | K                    | Joback Method  |
| tc            | 744.07  | K                    | Joback Method  |
| tf            | 347.36  | K                    | Joback Method  |
| vc            | 0.489   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 307.02 | J/mol×K | 508.74          | Joback Method |
| cpg           | 324.02 | J/mol×K | 547.96          | Joback Method |
| cpg           | 339.61 | J/mol×K | 587.18          | Joback Method |
| cpg           | 354.06 | J/mol×K | 626.40          | Joback Method |
| cpg           | 367.63 | J/mol×K | 665.63          | Joback Method |
| cpg           | 380.59 | J/mol×K | 704.85          | Joback Method |
| cpg           | 393.20 | J/mol×K | 744.07          | 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=C22516105&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C22516105&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>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>rinpola:</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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