

# 2-Acetyl-5-norbornene

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | 5-Acetyl-2-norbornene<br>Ethanone, 1-bicyclo[2.2.1]hept-5-en-2-yl-<br>Bicyclo[2.2.1]hept-2-ene, 5-acetyl-<br>Bicyclo[2.2.1]hept-5-ene, 2-acetyl-<br>methyl (8,9,10-trinorborn-5-en-2-yl) ketone |
| <b>Inchi:</b>               | InChI=1S/C9H12O/c1-6(10)9-5-7-2-3-8(9)4-7/h2-3,7-9H,4-5H2,1H3   |
| <b>InchiKey:</b>            | NIMLCWCLVJRPFY-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C9H12O  |
| <b>SMILES:</b>              | CC(=O)C1CC2C=CC1C2  |
| <b>Mol. weight [g/mol]:</b> | 136.19  |
| <b>CAS:</b>                 | 5063-03-6   |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 27.63   | kJ/mol  | Joback Method  |
| hf            | -164.79 | kJ/mol  | Joback Method  |
| hfus          | 17.13   | kJ/mol  | Joback Method  |
| hvap          | 42.36   | kJ/mol  | Joback Method  |
| log10ws       | -1.79   |         | Crippen Method |
| logp          | 1.788   |         | Crippen Method |
| mcvol         | 113.220 | ml/mol  | McGowan Method |
| pc            | 3337.38 | kPa     | Joback Method  |
| tb            | 471.43  | K       | Joback Method  |
| tc            | 684.15  | K       | Joback Method  |
| tf            | 270.00  | K       | Joback Method  |
| vc            | 0.436   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 253.18 | J/molxK | 471.43          | Joback Method |
| cpg           | 323.10 | J/molxK | 648.70          | Joback Method |
| cpg           | 310.98 | J/molxK | 613.25          | Joback Method |
| cpg           | 298.00 | J/molxK | 577.79          | Joback Method |

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 284.07    | J/molxK | 542.34 | Joback Method |
| cpg   | 269.16    | J/molxK | 506.88 | Joback Method |
| cpg   | 334.40    | J/molxK | 684.15 | Joback Method |
| dvisc | 0.0008335 | Paxs    | 471.43 | Joback Method |
| dvisc | 0.0008670 | Paxs    | 437.86 | Joback Method |
| dvisc | 0.0009077 | Paxs    | 404.29 | Joback Method |
| dvisc | 0.0009584 | Paxs    | 370.72 | Joback Method |
| dvisc | 0.0010228 | Paxs    | 337.14 | Joback Method |
| dvisc | 0.0011074 | Paxs    | 303.57 | Joback Method |
| dvisc | 0.0012230 | Paxs    | 270.00 | Joback Method |

## Pressure Dependent Properties

| Property code | Value  | Unit | Pressure [kPa] | Source       |
|---------------|--------|------|----------------|--------------|
| tbrp          | 358.20 | K    | 2.40           | NIST Webbook |

## 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=C5063036&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5063036&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>tb:</b>   | Normal Boiling Point Temperature  |
| <b>tbrp:</b> | Boiling point at reduced pressure |
| <b>tc:</b>   | Critical Temperature              |
| <b>tf:</b>   | Normal melting (fusion) point     |
| <b>vc:</b>   | Critical Volume                   |

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