

# Bicyclo[2.2.1]hept-5-ene-2-carboxylic acid

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | 5-Norbornene-2-carboxylic acid<br>Bicyclo[2.2.1]-5-heptene-2-carboxylic acid<br>Bicyclo(2.2.1)hept-2-ene-5-carboxylic acid<br>Norbornenecarboxylic acid |
| <b>Inchi:</b>               | InChI=1S/C8H10O2/c9-8(10)7-4-5-1-2-6(7)3-5/h1-2,5-7H,3-4H2,(H,9,10)   |
| <b>InchiKey:</b>            | FYGUSUBEMUKACF-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C8H10O2   |
| <b>SMILES:</b>              | O=C(O)C1CC2C=CC1C2  |
| <b>Mol. weight [g/mol]:</b> | 138.16  |
| <b>CAS:</b>                 | 120-74-1  |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -117.61 | kJ/mol  | Joback Method  |
| hf            | -296.38 | kJ/mol  | Joback Method  |
| hfus          | 18.63   | kJ/mol  | Joback Method  |
| hvap          | 56.81   | kJ/mol  | Joback Method  |
| log10ws       | -1.19   |         | Crippen Method |
| logp          | 1.283   |         | Crippen Method |
| mcvol         | 105.000 | ml/mol  | McGowan Method |
| pc            | 4200.18 | kPa     | Joback Method  |
| tb            | 540.73  | K       | Joback Method  |
| tc            | 742.39  | K       | Joback Method  |
| tf            | 319.55  | K       | Joback Method  |
| vc            | 0.400   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 263.31 | J/molxK | 540.73          | Joback Method |
| cpg           | 316.07 | J/molxK | 708.78          | Joback Method |
| cpg           | 306.91 | J/molxK | 675.17          | Joback Method |
| cpg           | 297.10 | J/molxK | 641.56          | Joback Method |
| cpg           | 286.60 | J/molxK | 607.95          | Joback Method |

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 275.36    | J/molxK | 574.34 | Joback Method |
| cpg   | 324.64    | J/molxK | 742.39 | Joback Method |
| dvisc | 0.0005680 | Paxs    | 540.73 | Joback Method |
| dvisc | 0.0007313 | Paxs    | 503.87 | Joback Method |
| dvisc | 0.0009798 | Paxs    | 467.00 | Joback Method |
| dvisc | 0.0013804 | Paxs    | 430.14 | Joback Method |
| dvisc | 0.0020738 | Paxs    | 393.28 | Joback Method |
| dvisc | 0.0033892 | Paxs    | 356.41 | Joback Method |
| dvisc | 0.0062035 | Paxs    | 319.55 | Joback Method |

## Pressure Dependent Properties

| Property code | Value         | Unit | Pressure [kPa] | Source       |
|---------------|---------------|------|----------------|--------------|
| tbrp          | 420.50 ± 1.50 | K    | 3.70           | NIST Webbook |

## Sources

|                        |   |
|------------------------|---|
| <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=C120741&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C120741&amp;Units=SI</a> |
| <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>                                 |

## 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>mvol:</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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