

# Benzodiazepine

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C9H8N2/c1-2-4-9-8(3-1)7-10-5-6-11-9/h1-7,11H |
| <b>InchiKey:</b>            | GUJAGMICFDYKNR-UHFFFAOYSA-N                           |
| <b>Formula:</b>             | C9H8N2  |
| <b>SMILES:</b>              | <chem>C1=CNc2ccccc2C=N1</chem>                        |
| <b>Mol. weight [g/mol]:</b> | 144.17  |
| <b>CAS:</b>                 | 12794-10-4  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 436.35  | kJ/mol               | Joback Method  |
| hf            | 301.13  | kJ/mol               | Joback Method  |
| hfus          | 22.75   | kJ/mol               | Joback Method  |
| hvap          | 52.68   | kJ/mol               | Joback Method  |
| log10ws       | -2.29   |                      | Crippen Method |
| logp          | 2.002   |                      | Crippen Method |
| mvol          | 114.410 | ml/mol               | McGowan Method |
| pc            | 4723.61 | kPa                  | Joback Method  |
| rinpol        | 1589.00 |                      | NIST Webbook   |
| tb            | 557.50  | K                    | Joback Method  |
| tc            | 824.48  | K                    | Joback Method  |
| tf            | 423.36  | K                    | Joback Method  |
| vc            | 0.431   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 259.97 | J/molxK | 557.50          | Joback Method |
| cpg           | 275.21 | J/molxK | 602.00          | Joback Method |
| cpg           | 289.23 | J/molxK | 646.49          | Joback Method |
| cpg           | 302.07 | J/molxK | 690.99          | Joback Method |
| cpg           | 313.76 | J/molxK | 735.49          | Joback Method |
| cpg           | 324.35 | J/molxK | 779.99          | Joback Method |
| cpg           | 333.89 | J/molxK | 824.48          | 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=C12794104&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C12794104&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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