

# Guanidine, 2-benzothiazolyl-

|                      |                                                                                       |
|----------------------|---------------------------------------------------------------------------------------|
| Other names:         | Benzothiazole guanidine<br>Guanidine, 2-benzothiazolyl-<br>benzothiazol-2-ylguanidine |
| Inchi:               | InChI=1S/C8H8N4S/c9-7(10)12-8-11-5-3-1-2-4-6(5)13-8/h1-4H,(H4,9,10,11,12)             |
| InchiKey:            | QMHWARSFUCGBJK-UHFFFAOYSA-N                                                           |
| Formula:             | C8H8N4S                                                                               |
| SMILES:              | N=C(N)Nc1nc2ccccc2s1                                                                  |
| Mol. weight [g/mol]: | 192.25                                                                                |

## Physical Properties

| Property code | Value   | Unit   | Source             |
|---------------|---------|--------|--------------------|
| ie            | 7.96    | eV     | Cheméo Relay (1.0) |
| log10ws       | -3.10   |        | Cheméo Relay (1.0) |
| logp          | 1.602   |        | Crippen Method     |
| mcvol         | 136.630 | ml/mol | McGowan Method     |
| tb            | 603.27  | K      | Cheméo Relay (1.0) |
| tf            | 503.68  | K      | Cheméo Relay (1.0) |

## Sources

|                           |                                                                                                                                             |
|---------------------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method:           | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                   |
| Crippen Method:           | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                           |
| Cheméo Relay (1.0):       |                                                                                                                                             |
| Cheméo Relay (1.0, beta): |                                                                                                                                             |
| NIST Webbook:             | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2582072&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2582072&amp;Units=SI</a> |
| McGowan Method:           | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                       |

## Legend

|          |                                    |
|----------|------------------------------------|
| ie:      | Ionization energy                  |
| log10ws: | Log10 of Water solubility in mol/l |

|               |                                     |
|---------------|-------------------------------------|
| <b>logp:</b>  | Octanol/Water partition coefficient |
| <b>mcvol:</b> | McGowan's characteristic volume     |
| <b>tb:</b>    | Normal Boiling Point Temperature    |
| <b>tf:</b>    | Normal melting (fusion) point       |

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