

# 3-Bromo-1H-1,2,4-triazole

|                      |                                                                                                           |
|----------------------|-----------------------------------------------------------------------------------------------------------|
| Other names:         | s-Triazole, 3-bromo-<br>3-Bromo-1,2,4-triazole<br>3-Bromo-1H-1,2,4-triazole<br>1H-1,2,4-Triazole,5-bromo- |
| Inchi:               | InChI=1S/C2H2BrN3/c3-2-4-1-5-6-2/h1H,(H,4,5,6)                                                            |
| InchiKey:            | HHIZISRHAQPAMY-UHFFFAOYSA-N                                                                               |
| Formula:             | C2H2BrN3                                                                                                  |
| SMILES:              | Brc1nc[nH]n1                                                                                              |
| Mol. weight [g/mol]: | 147.96                                                                                                    |

## Physical Properties

| Property code | Value  | Unit   | Source             |
|---------------|--------|--------|--------------------|
| ie            | 9.90   | eV     | NIST Webbook       |
| log10ws       | -0.42  |        | Cheméo Relay (1.0) |
| logp          | 0.085  |        | Crippen Method     |
| mcvol         | 67.020 | ml/mol | McGowan Method     |
| tf            | 392.41 | K      | Cheméo Relay (1.0) |

## Sources

|                           |                                                                                                                                             |
|---------------------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| NIST Webbook:             | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C7343331&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C7343331&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>                       |
| 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): |                                                                                                                                             |

## Legend

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

**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**tf:** Normal melting (fusion) point

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