

# Benzothiazol-2-ylacetonitrile

|                      |                                                            |
|----------------------|------------------------------------------------------------|
| Other names:         | Benzothiazol-2-ylacetonitrile                              |
| Inchi:               | InChI=1S/C9H6N2S/c10-6-5-9-11-7-3-1-2-4-8(7)12-9/h1-4H,5H2 |
| InchiKey:            | ZMZSYUSDGRJZNT-UHFFFAOYSA-N                                |
| Formula:             | C9H6N2S                                                    |
| SMILES:              | N#CCc1nc2ccccc2s1                                          |
| Mol. weight [g/mol]: | 174.23                                                     |

## Physical Properties

| Property code | Value   | Unit   | Source             |
|---------------|---------|--------|--------------------|
| ie            | 9.01    | eV     | Cheméo Relay (1.0) |
| log10ws       | -2.48   |        | Cheméo Relay (1.0) |
| logp          | 2.362   |        | Crippen Method     |
| mcvol         | 126.460 | ml/mol | McGowan Method     |
| tb            | 590.35  | K      | Cheméo Relay (1.0) |
| tf            | 395.14  | 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=C56278503&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C56278503&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  |
| logp:    | Octanol/Water partition coefficient |
| mcvol:   | McGowan's characteristic volume     |

**tb:** Normal Boiling Point Temperature

**tf:** Normal melting (fusion) point

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