# 2-Benzothiazolamine

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|---|---|
| **Other names:** | 2(3H)-Benzothiazolimine |
| | 2-Aminobenzthiazole |
| | 2-Benzothiazolylamine |
| | 2-Iminobenzothiazoline |
| | 2-aminobenzo[d]thiazole |
| | 2-aminobenzothiazole |
| | Benzothiazol-2-ylamine |
| | Benzothiazole, 2-amino- |
| | NSC 4670 |
| | USAF EK-3941 |
| | USAF XR-27 |
| | o-Aminobenzothiazole |
| **Inchi:** | InChI=1S/C7H6N2S/c8-7-9-5-3-1-2-4-6(5)10-7/h1-4H,(H2,8,9) |
| **InchiKey:** | UHGULLIUJBCTEF-UHFFFAOYSA-N |
| **Formula:** | C7H6N2S |
| **SMILES:** | Nc1nc2ccccc2s1 |
| **Mol. weight [g/mol]:** | 150.20 |
| **CAS:** | 136-95-8 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -2.43 | | Crippen Method |
| logp | 1.878 | | Crippen Method |
| mcvol | 106.880 | ml/mol | McGowan Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|

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| cps | 153.21 | J/mol×K | 298.15 | Standard enthalpies of formation of 2-aminobenzothiazoles in the crystalline phase by rotating-bomb combustion calorimetry |
| hvapt | 102.10 | kJ/mol | 298.15 | Thermodynamic study of 2-aminothiazole and 2-aminobenzothiazole: Experimental and computational approaches |

# Sources

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|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Standard enthalpies of formation of 2-aminobenzothiazoles in the crystalline phase by rotating-bomb combustion calorimetry:** | https://www.doi.org/10.1016/j.jct.2014.01.018 |
| **Thermodynamic study of 2-aminothiazole and 2-aminobenzothiazole: Experimental and computational approaches:** | https://www.doi.org/10.1016/j.jct.2014.04.001 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C136958&Units=SI |

# Legend

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| **cps:** | Solid phase heat capacity |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |