# (2-Benzimidazolylthio)-acetic acid

**Inchi:** InChI=1S/C9H8N2O2S/c12-8(13)5-14-9-10-6-3-1-2-4-7(6)11-9/h1-4H,5H2,(H,10,11)(H,1
**InchiKey:** UYNVBLJQBCTRKV-UHFFFAOYSA-N
**Formula:** C9H8N2O2S
**SMILES:** O=C(O)CSc1nc2ccccc2[nH]1
**Mol. weight [g/mol]:** 208.24

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -2.66 | | Cheméo Relay (1.0) |
| logp | 1.258 | | Crippen Method |
| mcvol | 142.500 | ml/mol | McGowan Method |
| tf | 518.49 | K | Cheméo Relay (1.0) |

## Sources

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws
**Cheméo Relay (1.0):**
**Cheméo Relay (1.0, beta):**
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C3042000&Units=SI
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

## Legend

**log10ws:** Log10 of Water solubility in mol/l
**logp:** Octanol/Water partition coefficient
**mcvol:** McGowan's characteristic volume
**tf:** Normal melting (fusion) point

Latest version available from:
https://www.chemeo.com/cid/28-239-6/2-Benzimidazolylthio-acetic-acid.pdf