# PROTHIONAMIDE

**Inchi:** InChI=1S/C9H12N2S/c1-2-3-8-6-7(9(10)12)4-5-11-8/h4-6H,2-3H2,1H3,(H2,10,12)
**InchiKey:** VRDIULHPQTYCLN-UHFFFAOYSA-N
**Formula:** C9H12N2S
**SMILES:** CCCc1cc(C(N)=S)ccn1
**Mol. weight [g/mol]:** 180.28

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| logp | 1.668 | | Crippen Method |
| mcvol | 145.920 | ml/mol | McGowan Method |
| tb | 576.27 | K | Cheméo Relay (1.0) |
| tf | 416.85 | K | Cheméo Relay (1.0) |

## Sources

**Cheméo Relay (1.0, beta):**
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?Str2File=C14222607
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**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):**

## Legend

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