# 2-Benzothiazolinethione, 3-(4-nitrophenylaminomethyl)-

**Inchi:** InChI=1S/C14H11N3O2S2/c18-17(19)11-7-5-10(6-8-11)15-9-16-12-3-1-2-4-13(12)21-14

**InchiKey:** UTKZLNADJQUIFU-UHFFFAOYSA-N

**Formula:** C14H11N3O2S2

**SMILES:** O=[N+]([O-])c1ccc(NCn2c(=S)sc3ccccc32)cc1

**Mol. weight [g/mol]:** 317.39

**CAS:** 60431-65-4

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -6.11 | | Crippen Method |
| logp | 4.410 | | Crippen Method |
| mcvol | 215.520 | ml/mol | McGowan Method |

## Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C60431654&Units=SI

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

## Legend

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume