

# Adenine, n-[p-(methylthio)phenyl]-

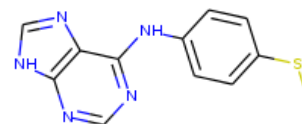
**InChI:** InChI=1S/C12H11N5S/c1-18-9-4-2-8(3-5-9)17-12-10-11(14-6-13-10)15-7-16-12/h2-7H,1H3,(H2,13,14,15,16,17)

**InChI Key:** RLIKBBNNCGQLQX-UHFFFAOYSA-N

**Formula:** C12H11N5S

**SMILES:** CSc1ccc(Nc2ncnc3[nH]cnc32)cc1

**Molecular Weight:** 257.31



## Physical Properties

| Property                  | Value | Unit | Source         |
|---------------------------|-------|------|----------------|
| $\log P_{\text{oct/wat}}$ | 2.818 |      | Crippen Method |

## Sources

**NIST Webbook:** [http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H11N5S/c1-18-9-4-2-8\(3-5-9\)17-12-10-11\(14-6-13-10\)15-7-16-12/h2-7H,1H3,\(H2,13,14,15,16,17\)](http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H11N5S/c1-18-9-4-2-8(3-5-9)17-12-10-11(14-6-13-10)15-7-16-12/h2-7H,1H3,(H2,13,14,15,16,17))

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

$\log P_{\text{oct/wat}}$ : Octanol/Water partition coefficient .

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