# 9H-purine, 6-[(2-mercaptoethyl)thio]-, s-acetate

**Inchi:** InChI=1S/C9H10N4OS2/c1-6(14)15-2-3-16-9-7-8(11-4-10-7)12-5-13-9/h4-5H,2-3H2,1H3
**InchiKey:** CIJAISDDQRVOBA-UHFFFAOYSA-N
**Formula:** C9H10N4OS2
**SMILES:** CC(=O)SCCSc1ncnc2[nH]cnc12
**Mol. weight [g/mol]:** 254.33

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -3.45 | | Crippen Method |
| logp | 1.243 | | Crippen Method |
| mcvol | 172.940 | ml/mol | McGowan Method |

## Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=B6008692&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws
**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