

# 9H-purine, 6-chloro-9-ethyl-

**InChI:**

InChI=1S/C7H7ClN4/c1-2-12-4-11-5-6(8)9-3-10-7(5)12/h3-4H,2H2,1H3

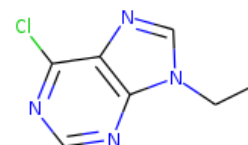
**InChI Key:** YSKHRCGNQFWRFM-UHFFFAOYSA-N

**Formula:** C7H7ClN4

**SMILES:** CCn1cnc2c1ncnc2Cl

**Molecular Weight:** 182.61

**CAS:** 5462-86-2



## Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	1.500		Crippen Method

## Sources

**NIST Webbook:**

[http://webbook.nist.gov/cgi/inchi/InChI=1S/C7H7ClN4/c1-2-12-4-11-5-6\(8\)9-3-10-7\(5\)12/h3-4H,2H2,1H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C7H7ClN4/c1-2-12-4-11-5-6(8)9-3-10-7(5)12/h3-4H,2H2,1H3)

**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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