

# 4-Hydroxyantipyrene

**Inchi:** InChI=1S/C11H12N2O2/c1-8-10(14)11(15)13(12(8)2)9-6-4-3-5-7-9/h3-7,14H,1-2H3  
**InchiKey:** SKVPTPMWXJSBTF-UHFFFAOYSA-N  
**Formula:** C11H12N2O2  
**SMILES:** Cc1c(O)c(=O)n(-c2ccccc2)n1C  
**Mol. weight [g/mol]:** 204.23  
**CAS:** 1672-63-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.86		Crippen Method
logp	1.190		Crippen Method
mcvol	154.330	ml/mol	McGowan Method
rinpol	1873.00		NIST Webbook
rinpol	1873.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1672635&Units=SI>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpol:** Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/124-198-5/4-Hydroxyantipyrene.pdf>

Generated by Cheméo on 2024-05-02 20:32:17.325476941 +0000 UTC m=+16971186.246054254.  
Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.