

# 6-methoxypteridine

**Inchi:** InChI=1S/C7H6N4O/c1-12-6-3-9-7-5(11-6)2-8-4-10-7/h2-4H,1H3  
**InchiKey:** AWIJPALBOQNRBS-UHFFFAOYSA-N  
**Formula:** C7H6N4O  
**SMILES:** COc1cnc2ncncc2n1  
**Mol. weight [g/mol]:** 162.15

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.14		Estimated Solubility Method
logp	0.428		Crippen Method
mcvol	112.060	ml/mol	McGowan Method

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Estimated Solubility Method:** [http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl\\_file/ci034243xsi20040112\\_053635.txt](http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt)  
**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

Latest version available from:

<https://www.cheméo.com/cid/104-736-9/6-methoxypteridine.pdf>

Generated by Cheméo on 2024-05-06 19:46:41.159701914 +0000 UTC m=+17314050.080279226.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.