

# MEPANIPYRIM

**Other names:** 2-Pyrimidinamine, 4-methyl-N-phenyl-6-(1-propyn-1-yl)-  
**Inchi:** InChI=1S/C14H13N3/c1-3-7-13-10-11(2)15-14(17-13)16-12-8-5-4-6-9-12/h4-6,8-10H,1-2  
**InchiKey:** CIFWZNRJIBNXRE-UHFFFAOYSA-N  
**Formula:** C14H13N3  
**SMILES:** CC#Cc1cc(C)nc(Nc2ccccc2)n1  
**Mol. weight [g/mol]:** 223.27  
**CAS:** 110235-47-7

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.40		Crippen Method
logp	2.900		Crippen Method
mcvol	181.940	ml/mol	McGowan Method
rinpol	2134.00		NIST Webbook
rinpol	2141.00		NIST Webbook
rinpol	2134.00		NIST Webbook

## Sources

**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=C110235477&Units=SI>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## Legend

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

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