

# 1H-pyrazolo[3,4-d]pyrimidine, 4-amino-1-methyl-

Inchi:	InChI=1S/C6H7N5/c1-11-6-4(2-10-11)5(7)8-3-9-6/h2-3H,1H3,(H2,7,8,9)
InchiKey:	JBMTUXVKTGBMLE-UHFFFAOYSA-N
Formula:	C6H7N5
SMILES:	Cn1ncc2c(N)ncnc21
Mol. weight [g/mol]:	149.15
CAS:	5334-99-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.49		Crippen Method
logp	-0.054		Crippen Method
mcvol	106.380	ml/mol	McGowan Method

## Sources

Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C5334996&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5334996&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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