

# 1H-1,2,4-Triazole, 3,5-dimethyl-

**Inchi:** InChI=1S/C4H7N3/c1-3-5-4(2)7-6-3/h1-2H3,(H,5,6,7)  
**InchiKey:** XYYXDARQOHWBPO-UHFFFAOYSA-N  
**Formula:** C4H7N3  
**SMILES:** Cc1n[nH]c(C)n1  
**Mol. weight [g/mol]:** 97.12  
**CAS:** 7343-34-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.17		Crippen Method
logp	-0.060		Crippen Method
mcvol	77.700	ml/mol	McGowan Method
tb	531.70	K	NIST Webbook

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	432.20	K	2.50	NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C7343342&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307I>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure

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