

# 4,5,6,7-Tetrahydropyrazolo[1,5-d][1,2,4]-triazin-4-one-2,6,7,7-tetramethyl

InChI: CN1C=NC2C(C1)C(O)=NN(C)C2(C)C  
InChIKey: WPBAKWWCBWRZED-UHFFFAOYSA-N

Formula: C<sub>9</sub>H<sub>16</sub>N<sub>4</sub>O  
SMILES: CC1=NN2C(C1)C(O)=NN(C)C2(C)C  
Mol. weight [g/mol]: 196.25

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.37		Crippen Method
logp	0.990		Crippen Method
mcvol	153.140	ml/mol	McGowan Method

## Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R582340&Units=SI>  
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>

## 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.chemeo.com/cid/98-820-3/4-5-6-7-Tetrahydropyrazolo-1-5-d-1-2-4-triazin-4-one-2-6-7-7-tetramethyl.pdf>

Generated by Cheméo on 2024-05-03 17:03:40.063302431 +0000 UTC m=+17045068.983879746.

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