

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

InChI: Cc1c2c(c1)nc(=O)nn2C(C)C(C)C(C)C(C)C  
InChIKey: GIQCMCKCJUOTGZ-UHFFFAOYSA-N  
Formula: C<sub>11</sub>H<sub>18</sub>N<sub>4</sub>O  
SMILES: CC1=NN2C(C1)C(=O)NN(C)C21CCCC1  
Mol. weight [g/mol]: 222.29

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.08		Crippen Method
logp	0.684		Crippen Method
mcvol	170.460	ml/mol	McGowan Method
rinpola	1853.00		NIST Webbook

## Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
Crippen Method: [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.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=R582375&Units=SI>

## Legend

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

Latest version available from:

<https://www.cheméo.com/cid/38-174-7/4-5-6-7-Tetrahydropyrazolo-1-5-d-1-2-4-triazin-4-one-2-6-dimethyl-7-7-tetramethylene>

Generated by Cheméo on 2024-04-25 14:39:03.423960876 +0000 UTC m=+16345192.344538192.

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