

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

InChI: Cc1c(C)c(C)nc(=O)n1C  
InChIKey: MYSYXRWQWJHUFD-UHFFFAOYSA-N  
Formula: C<sub>13</sub>H<sub>22</sub>N<sub>4</sub>O  
SMILES: CC1=NN2C(C1)C(=O)N(C)N(C)C21CCCCC1  
Mol. weight [g/mol]: 250.34

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.30		Crippen Method
logp	1.416		Crippen Method
mcvol	198.640	ml/mol	McGowan Method
rinpol	1939.00		NIST Webbook
rinpol	1939.00		NIST Webbook

## Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
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=R582251&Units=SI>

## 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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