

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

InChI: CN1=NC2CN(C)NC(=O)C2C1

InChIKey: WBIBIFZCORZKHJ-UHFFFAOYSA-N

Formula: C7H12N4O

SMILES: CC1=NN2CN(C)NC(=O)C2C1

Mol. weight [g/mol]: 168.20

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.40		Crippen Method
logp	-0.629		Crippen Method
mcvol	124.960	ml/mol	McGowan Method
rinpole	1544.00		NIST Webbook

## Sources

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>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R582355&Units=SI>

## Legend

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

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