

# 1,2,3-Benzotriazin-4(1H)-one

<b>Other names:</b>	1,2,3-Benzotriazin-4(3H)-one Benzazimide Benzazimidone 1,2,3-Benzotriazin-4-ol 4-Ketobenz-1,2,3-triazine 4-Ketobenzotriazine USAF MA-2 4-Ketobenzotriazine Benzoketotriazine 3H-1,2,3-Benzotriazin-4-one NSC 13563
<b>Inchi:</b>	InChI=1S/C7H5N3O/c11-7-5-3-1-2-4-6(5)8-10-9-7/h1-4H,(H,8,9,11)
<b>InchiKey:</b>	DMSSTTLDFWKBSX-UHFFFAOYSA-N
<b>Formula:</b>	C7H5N3O
<b>SMILES:</b>	O=c1nn[nH]c2ccccc12
<b>Mol. weight [g/mol]:</b>	147.13
<b>CAS:</b>	90-16-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.45		Crippen Method
logp	-0.164		Crippen Method
mcvol	102.080	ml/mol	McGowan Method

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C90164&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C90164&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

# Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume

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