

# 1,2,3-Benzotriazine-4(3h)-one, 6-chloro-

<b>Inchi:</b>	InChI=1S/C7H4ClN3O/c8-4-1-2-6-5(3-4)7(12)10-11-9-6/h1-3H,(H,9,10,12)
<b>InchiKey:</b>	ICRNYWUEKICFMZ-UHFFFAOYSA-N
<b>Formula:</b>	C7H4ClN3O
<b>SMILES:</b>	O=c1[nH]nnc2ccc(Cl)cc12
<b>Mol. weight [g/mol]:</b>	181.58
<b>CAS:</b>	37429-97-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.13		Crippen Method
logp	0.490		Crippen Method
mcvol	114.320	ml/mol	McGowan Method

## Sources

<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>
<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=C37429973&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C37429973&amp;Units=SI</a>

## Legend

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

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