

# 2(3H)-Benzothiazolone

<b>Other names:</b>	2-Benzothiazolinone Benzothiazolone Carbamothioic acid, (2-mercatophenyl)-, «gamma»-lactone 2-Benzothiazolol 2-Hydroxybenzothiazole 2-Benzothiazolone Benzothiazol, 2-hydroxy- 2-Benzothiazolol (keto form) benzothiazol-2(3H)-one
<b>Inchi:</b>	InChI=1S/C7H5NOS/c9-7-8-5-3-1-2-4-6(5)10-7/h1-4H,(H,8,9)
<b>InchiKey:</b>	YEDUAINPPJYDJZ-UHFFFAOYSA-N
<b>Formula:</b>	C7H5NOS
<b>SMILES:</b>	O=c1[nH]c2ccccc2s1
<b>Mol. weight [g/mol]:</b>	151.19
<b>CAS:</b>	934-34-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.67		Crippen Method
logp	1.108		Crippen Method
mcvol	102.770	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=C934349&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C934349&amp;Units=SI</a>

## Legend

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

Latest version available from:

<https://www.cheméo.com/cid/57-054-9/2-3H-Benzothiazolone.pdf>

Generated by Cheméo on 2024-04-23 09:15:51.417658882 +0000 UTC m=+16153000.338236197.

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