

# Acetic acid, (2-benzothiazolyloxy)-

<b>Other names:</b>	2-Benzothiazolyloxy acetic acid
<b>Inchi:</b>	InChI=1S/C9H7NO3S/c11-8(12)5-13-9-10-6-3-1-2-4-7(6)14-9/h1-4H,5H2,(H,11,12)
<b>InchiKey:</b>	OPQIOIYLAKHILI-UHFFFAOYSA-N
<b>Formula:</b>	C9H7NO3S
<b>SMILES:</b>	O=C(O)COc1nc2ccccc2s1
<b>Mol. weight [g/mol]:</b>	209.22
<b>CAS:</b>	2875-32-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.44		Crippen Method
logp	1.760		Crippen Method
mcvol	138.390	ml/mol	McGowan Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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=C2875323&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2875323&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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