

# 1,2-Benzisoxazole

<b>Other names:</b>	Indoxazene 1-Oxa-2-azaindene 1-Oxa-2-aza-1H-indene 4,5-Benzisoxazole 4,5-Benzisoazole benz[d]isoxazole
<b>Inchi:</b>	InChI=1S/C7H5NO/c1-2-4-7-6(3-1)5-8-9-7/h1-5H
<b>InchiKey:</b>	KTZQTRPPVKQPFO-UHFFFAOYSA-N
<b>Formula:</b>	C7H5NO
<b>SMILES:</b>	c1ccc2oncc2c1
<b>Mol. weight [g/mol]:</b>	119.12
<b>CAS:</b>	271-95-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.78		Crippen Method
logp	1.828		Crippen Method
mcvol	86.420	ml/mol	McGowan Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	364.20	K	2.00	NIST Webbook

## 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=C271954&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C271954&amp;Units=SI</a>
<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>

# Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcpvol:</b>	McGowan's characteristic volume
<b>tbrp:</b>	Boiling point at reduced pressure

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