

# 2,1,3-Benzoselenadiazole

<b>Other names:</b>	Benzo-2,1,3-selenadiazole Piaselenole Piazselenol Piazselenole 2-Selena-1,3-diaza-2H-isoindene 3,4-Benzo-1,2,5-selenadiazole
<b>Inchi:</b>	InChI=1S/C6H4N2Se/c1-2-4-6-5(3-1)7-9-8-6/h1-4H
<b>InchiKey:</b>	AYTPIVIDHMGVGSX-UHFFFAOYSA-N
<b>Formula:</b>	C6H4N2Se
<b>SMILES:</b>	<chem>c1ccc2n[se]nc2c1</chem>
<b>Mol. weight [g/mol]:</b>	183.07
<b>CAS:</b>	273-15-4

## Physical Properties

Property code	Value	Unit	Source
ie	8.76	eV	NIST Webbook
log10ws	0.07		Crippen Method
logp	0.687		Crippen Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C273154&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C273154&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient

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