# 2,1,3-Benzoselenadiazole

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

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C273154&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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|---|---|
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |