

Benzoselenadiazole, 2,1,3-

Inchi: InChI=1S/C6H4N2Se/c1-2-4-6-5(3-1)7-9-8-6/h1-4H
InchiKey: AYTPIVIDHMGVSX-UHFFFAOYSA-N
Formula: C6H4N2Se
SMILES: c1ccc2n[se]nc2c1
Mol. weight [g/mol]: 183.07
CAS: 22706-23-6

Physical Properties

Property code	Value	Unit	Source
log10ws	0.07		Crippen Method
logp	0.687		Crippen Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C22706236&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient

Latest version available from:

<https://www.cheméo.com/cid/98-582-8/Benzoselenadiazole-2-1-3.pdf>

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