

[1,2,5]Selenadiazolo[3,4-d]pyrimidin-7(6h)-one

Inchi: InChI=1S/C4H2N4OSe/c9-4-2-3(5-1-6-4)8-10-7-2/h1H,(H,5,6,8,9)
InchiKey: DYOWSWWSVPQCPE-UHFFFAOYSA-N
Formula: C4H2N4OSe
SMILES: O=c1[nH]cnc2n[se]nc12
Mol. weight [g/mol]: 201.04
CAS: 7698-94-4

Physical Properties

Property code	Value	Unit	Source
log10ws	1.66		Crippen Method
logp	-1.712		Crippen Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C7698944&Units=SI>

Legend

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

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