

# Panidazole

**Inchi:** InChI=1S/C11H12N4O2/c1-9-13-8-11(15(16)17)14(9)7-4-10-2-5-12-6-3-10/h2-3,5-6,8H,4  
**InchiKey:** ARYPMCPJIWUCIP-UHFFFAOYSA-N  
**Formula:** C11H12N4O2  
**SMILES:** Cc1ncc([N+](=O)[O-])n1CCc1ccncc1  
**Mol. weight [g/mol]:** 232.24  
**CAS:** 13752-33-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.01		Crippen Method
logp	1.737		Crippen Method
mcvol	169.990	ml/mol	McGowan Method
rinpol	2065.00		NIST Webbook
rinpol	2065.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C13752335&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpol:** Non-polar retention indices

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