

# Pinazepam

**Other names:**

2H-1,4-Benzodiazepin-2-one, 7-chloro-1,3-dihydro-5-phenyl-1-(2-propynyl)-Zami 905  
2H-1,4-Benzodiazepin-2-one, 1,3-dihydro-7-chloro-5-phenyl-1-(2-propynyl)-7-Chloro-1,3-dihydro-5-phenyl-1-(2-propynyl)-2H-1,4-benzodiazepin-2-one  
7-Chloro-1-propargyl-5-phenyl-2H-1,4-benzodiazepin-2-one  
Domar  
Z-905  
Duna

**Inchi:**

InChI=1S/C18H13ClN2O/c1-2-10-21-16-9-8-14(19)11-15(16)18(20-12-17(21)22)13-6-4-3

**InchiKey:**

MFZOSKPPVCIFMT-UHFFFAOYSA-N

**Formula:**

C<sub>18</sub>H<sub>13</sub>ClN<sub>2</sub>O

**SMILES:**

C#CCN1C(=O)CN=C(c2ccccc2)c2cc(Cl)ccc21

**Mol. weight [g/mol]:**

308.76

**CAS:**

52463-83-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.15		Crippen Method
logp	3.157		Crippen Method
mcvol	226.970	ml/mol	McGowan Method
rinpol	2529.00		NIST Webbook
rinpol	2580.00		NIST Webbook
rinpol	2572.00		NIST Webbook
rinpol	2551.00		NIST Webbook
rinpol	2531.00		NIST Webbook
rinpol	2551.00		NIST Webbook
rinpol	2529.00		NIST Webbook
rinpol	2580.00		NIST Webbook
rinpol	2572.00		NIST Webbook
rinpol	2529.00		NIST Webbook
rinpol	2551.00		NIST Webbook
rinpol	2529.00		NIST Webbook

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C52463839&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C52463839&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307i">http://pubs.acs.org/doi/abs/10.1021/ci990307i</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

# Legend

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

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