

# Phosphorothioic acid, O-(1,6-dihydro-6-oxo-1-phenyl-3-pyridazinyl) O,O-diethyl ester

Other names:

Pyridaphenthion

Phosphorothioic acid, O,O-diethyl ester, O-ester with 6-hydroxy-2-phenyl-3(2H)-pyridazinone  
American cyanamid 12,503

CL 12503

O,O-Diethyl O-(2,3-dihydro-3-oxo-2-phenyl-6-pyridazinyl)phosphorothioate

O,O-Diethylphosphorothioate, O-ester with 6-hydroxy-2-phenyl-3(2H)-pyridazinone

O-(1,6-Dihydro-6-oxo-1-phenylpyridazin-3-yl) O,O-diethyl phosphorothioate

ENT 23,968

Ofnack

Ofnak

Ofunack

Pyridaphenthion

3(2H)-Pyridazinone, 6-hydroxy-2-phenyl-, O-ester with O,O-diethyl

phosphorothioate

O,O-diethyl O-(1,6-dihydro-6-oxo-1-phenylpyridazin-3-yl) thiophosphate

**Inchi:**

InChI=1S/C14H17N2O4PS/c1-3-18-21(22,19-4-2)20-13-10-11-14(17)16(15-13)12-8-6-5-

**InchiKey:**

CXJSOEPQXUCJSA-UHFFFAOYSA-N

**Formula:**

C14H17N2O4PS

**SMILES:**

CCOP(=S)(OCC)Oc1ccc(=O)n(-c2ccccc2)n1

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

340.33

**CAS:**

119-12-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.12		Crippen Method
logp	2.909		Crippen Method
mcvol	240.850	ml/mol	McGowan Method
rinpol	2455.00		NIST Webbook
rinpol	2437.00		NIST Webbook
rinpol	2450.00		NIST Webbook
rinpol	2418.00		NIST Webbook
rinpol	2437.00		NIST Webbook
rinpol	2478.00		NIST Webbook

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C119120&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C119120&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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