

# Diazoxon

<b>Other names:</b>	Phosphoric acid, diethyl 6-methyl-2-(1-methylethyl)-4-pyrimidinyl ester Phosphoric acid, diethyl 2-isopropyl-6-methyl-4-pyrimidinyl ester Diazinon oxon Oxodiazinon Diazinon O-analog
<b>Inchi:</b>	InChI=1S/C12H21N2O4P/c1-6-16-19(15,17-7-2)18-11-8-10(5)13-12(14-11)9(3)4/h8-9H,6
<b>InchiKey:</b>	VBLJFQYCTRKKKF-UHFFFAOYSA-N
<b>Formula:</b>	C12H21N2O4P
<b>SMILES:</b>	CCOP(=O)(OCC)Oc1cc(C)nc(C(C)C)n1
<b>Mol. weight [g/mol]:</b>	288.28
<b>CAS:</b>	962-58-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.48		Crippen Method
logp	3.468		Crippen Method
mcvol	220.080	ml/mol	McGowan Method
rinpol	1766.00		NIST Webbook
rinpol	1732.00		NIST Webbook
rinpol	1732.00		NIST Webbook
rinpol	1766.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C962583&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C962583&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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

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

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