

# Isazophos

**Other names:** Isazofos  
Isozophos

**Inchi:** InChI=1S/C9H17CIN3O3PS/c1-5-14-17(18,15-6-2)16-9-11-8(10)13(12-9)7(3)4/h7H,5-6H

**InchiKey:** XRHGWAGWAHHFLF-UHFFFAOYSA-N

**Formula:** C9H17CIN3O3PS

**SMILES:** CCOP(=S)(OCC)Oc1nc(Cl)n(C(C)C)n1

**Mol. weight [g/mol]:** 313.74

**CAS:** 65357-77-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.14		Crippen Method
logp	3.189		Crippen Method
mcvol	214.810	ml/mol	McGowan Method
rinpol	1815.00		NIST Webbook
rinpol	1815.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C65357779&Units=SI>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## 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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