

Phosphorothioic acid, O-[5-chloro-1-(1-methylethyl)-1H-1,2,4-triazol-3-yl] O,O-diethyl ester

Other names:

Isazophos
ISAZOFUS

O-(5-chloro-1-isopropyl-1,2,4-triazol-3-yl) O,O-diethyl phosphorothioate

Inchi:	InChI=1S/C9H17ClN3O3PS/c1-5-14-17(18,15-6-2)16-9-11-8(10)13(12-9)7(3)4/h7H,5-6H
InchiKey:	XRHWAGWAHFLF-UHFFFAOYSA-N
Formula:	C9H17ClN3O3PS
SMILES:	CCOP(=S)(OCC)Oc1nc(Cl)n(C(C)C)n1
Mol. weight [g/mol]:	313.74
CAS:	42509-80-8

Physical Properties

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

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C42509808&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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