

# fosthiazate-1

<b>Other names:</b>	Fostiazate, isomer 1 FOSTHIAZATE-2 Phosphonothioic acid, P-(2-oxo-3-thiazolidinyl)-, O-ethyl S-(1-methylpropyl) ester fosthiazate O-ethyl S-(1-methylpropyl) (2-oxo-3-thiazolidinyl)phosphonothioate Fostiazate, isomer 2
<b>Inchi:</b>	InChI=1S/C9H18NO3PS2/c1-4-8(3)16-14(12,13-5-2)10-6-7-15-9(10)11/h8H,4-7H2,1-3H3
<b>InchiKey:</b>	DUFVKSUJRWYZQP-UHFFFAOYSA-N
<b>Formula:</b>	C9H18NO3PS2
<b>SMILES:</b>	CCOP(=O)(SC(C)CC)N1CCSC1=O
<b>Mol. weight [g/mol]:</b>	283.35

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.04		Crippen Method
logp	3.832		Crippen Method
mcvol	203.260	ml/mol	McGowan Method
rinpol	2027.00		NIST Webbook
rinpol	2032.00		NIST Webbook
rinpol	2032.00		NIST Webbook
rinpol	2027.00		NIST Webbook

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C98886443&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C98886443&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>

## 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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