

# 4-Oxo-2-thioxo-3-thiazolidineacetic acid, ethyl ester

<b>Inchi:</b>	InChI=1S/C7H9NO3S2/c1-2-11-6(10)3-8-5(9)4-13-7(8)12/h2-4H2,1H3
<b>InchiKey:</b>	QDRLGCJQLOXVLY-UHFFFAOYSA-N
<b>Formula:</b>	C7H9NO3S2
<b>SMILES:</b>	CCOC(=O)CN1C(=O)CSC1=S
<b>Mol. weight [g/mol]:</b>	219.28
<b>CAS:</b>	23176-01-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.09		Crippen Method
logp	0.410		Crippen Method
mcvol	146.020	ml/mol	McGowan Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C23176014&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C23176014&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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

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