

# 9H-purine, 6-mercapto-, 8-ethyl-

<b>Inchi:</b>	InChI=1S/C7H8N4S/c1-2-4-10-5-6(11-4)8-3-9-7(5)12/h3H,2H2,1H3,(H2,8,9,10,11,12)
<b>InchiKey:</b>	PZCCURWYGRJQAG-UHFFFAOYSA-N
<b>Formula:</b>	C7H8N4S
<b>SMILES:</b>	CCc1nc2c(S)ncnc2[nH]1
<b>Mol. weight [g/mol]:</b>	180.23
<b>CAS:</b>	101861-17-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.11		Crippen Method
logp	0.722		Crippen Method
mcvol	126.840	ml/mol	McGowan Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C101861170&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C101861170&amp;Units=SI</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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