

# Triazolo[4,5-d]pyrimidine, 3h-v-,5-amino-7-benzylthio-3-ethyl-

<b>Inchi:</b>	InChI=1S/C13H14N6S/c1-2-19-11-10(17-18-19)12(16-13(14)15-11)20-8-9-6-4-3-5-7-9/h
<b>InchiKey:</b>	WRUMIWLCVFKRPY-UHFFFAOYSA-N
<b>Formula:</b>	C13H14N6S
<b>SMILES:</b>	CCn1nnc2c(SCc3ccccc3)nc(=N)[nH]c21
<b>Mol. weight [g/mol]:</b>	286.36
<b>CAS:</b>	96229-34-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.90		Crippen Method
logp	1.464		Crippen Method
mcvol	207.580	ml/mol	McGowan Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C96229344&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C96229344&amp;Units=SI</a>
<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>

## 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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