

# Carbamic acid, thio-2-benzimidazole, ethyl ester

<b>Inchi:</b>	InChI=1S/C10H11N3OS/c1-2-14-10(15)13-9-11-7-5-3-4-6-8(7)12-9/h3-6H,2H2,1H3,(H2,
<b>InchiKey:</b>	KTPZQCLIIQJBJM-UHFFFAOYSA-N
<b>Formula:</b>	C10H11N3OS
<b>SMILES:</b>	CCOC(S)=Nc1nc2ccccc2[nH]1
<b>Mol. weight [g/mol]:</b>	221.28
<b>CAS:</b>	13404-88-1

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.40		Crippen Method
logp	2.035		Crippen Method
mcvol	160.700	ml/mol	McGowan Method

## 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=C13404881&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C13404881&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>

## 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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