

# 1,2,4-Triazin-5(2H)-one, 6-(1,1-dimethylethyl)-3-(methylthio)-

<b>Other names:</b>	Deaminated sencor Deaminometribuzin 6-(1,1-Dimethylethyl)-3-(methylthio)-1,2,4-triazin-5(2H)-one Metribuzin DA 6-tert-Butyl-3-(methylsulfanyl)-1,2,4-triazin-5(2H)-one Metribuzin, des-amino Desaminometribuzin Metribuzin M (des-amino)
<b>Inchi:</b>	InChI=1S/C8H13N3OS/c1-8(2,3)5-6(12)9-7(13-4)11-10-5/h1-4H3,(H,9,11,12)
<b>InchiKey:</b>	MIWRSUQXSCLDNLV-UHFFFAOYSA-N
<b>Formula:</b>	C8H13N3OS
<b>SMILES:</b>	CSc1nc(=O)c(C(C)(C)C)n[nH]1
<b>Mol. weight [g/mol]:</b>	199.27
<b>CAS:</b>	35045-02-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.70		Crippen Method
logp	0.702		Crippen Method
mvol	151.980	ml/mol	McGowan Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C35045024&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C35045024&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>
<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

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume

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