

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

**Other names:** 6-(1,1-Dimethylethyl)-3-(methylthio)-1,2,4-triazin-5(2H)-one

6-tert-Butyl-3-(methylsulfanyl)-1,2,4-triazin-5(2H)-one

Deaminated sencor

Deaminometribuzin

Desaminometribuzin

Metribuzin DA

Metribuzin M (des-amino)

Metribuzin, des-amino

**Inchi:** InChI=1S/C8H13N3OS/c1-8(2,3)5-6(12)9-7(13-4)11-10-5/h1-4H3,(H,9,11,12)

**InchiKey:** MIWRSUQXSCLDNV-UHFFFAOYSA-N

**Formula:** C8H13N3OS

**SMILES:** CSc1nc(=O)c(C(C)(C)C)n[nH]1

**Mol. weight [g/mol]:** 199.28

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| logp          | 0.702   |        | Crippen Method |
| mcvol         | 151.980 | ml/mol | McGowan Method |

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**Cheméo Relay (1.0):**

**Cheméo Relay (1.0, beta):**

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C35045024&Units=SI>

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## Legend

**logp:** Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume

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