

# 2E,4Z-Hexadiene, adduct with 4-methyl-1,2,4-triazolin-3,5-dione

**Other names:** 2E,4Z-Hexadiene + MTAD adduct  
**Inchi:** InChI=1S/C9H13N3O2/c1-6-4-5-7(2)12-9(14)10(3)8(13)11(6)12/h4-7H,1-3H3/t6-,7-/m1/s  
**InchiKey:** MJBCSCMWBFGHCJ-RNFRBKRXSA-N  
**Formula:** C9H13N3O2  
**SMILES:** CC1C=CC(C)n2c(=O)n(C)c(=O)n21  
**Mol. weight [g/mol]:** 195.22

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.64		Crippen Method
logp	0.040		Crippen Method
mcvol	144.730	ml/mol	McGowan Method
rinpola	1580.00		NIST Webbook
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## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U293258&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpola:** Non-polar retention indices

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