

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

Other names:	2E,4E-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+
InchiKey:	MJBCSCMWBFHGHCJ-KNVOCYPGSA-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

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U293257&Units=SI

Legend

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

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<https://www.chemeo.com/cid/16-701-5/2E-4E-Hexadiene-adduct-with-4-methyl-1-2-4-triazolin-3-5-dione.pdf>

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