

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

Other names:	1,3-Hexadiene + MTAD adduct
Inchi:	InChI=1S/C9H13N3O2/c1-3-7-5-4-6-11-8(13)10(2)9(14)12(7)11/h4-5,7H,3,6H2,1-2H3
InchiKey:	JFOAPFSYVHSUSW-UHFFFAOYSA-N
Formula:	C9H13N3O2
SMILES:	CCC1C=CCn2c(=O)n(C)c(=O)n21
Mol. weight [g/mol]:	195.22
CAS:	131916-23-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.68		Crippen Method
logp	-0.131		Crippen Method
mcvol	144.730	ml/mol	McGowan Method
rinpol	1680.00		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=C131916239&Units=SI

Legend

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

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