

Phosphoric acid, dimethyl 1-methyl-3-(methylamino)-3-oxo-1-propenyl ester, (Z)-

Other names: Phosphoric acid, dimethyl ester, ester with 3-hydroxy-N-methylcrotonamide, (Z)-
Phosphoric acid, dimethyl 1-methyl-3-(methylamino)-2-oxo-1-propenyl ester, (Z)-

Monocrotophos (Z)-analog

Dimethyl cis-1-methyl-2-methylcarbamoylvinyl phosphate

Dimethyl (1Z)-1-methyl-3-(methylamino)-3-oxo-1-propenyl phosphate

Azodrin, cis

cis-Azodrin

Monocrotophos

dimethyl (Z)-1-methyl-3-(methylamino)-3-oxoprop-1-enyl phosphate

Inchi: InChI=1S/C7H14NO5P/c1-6(5-7(9)8-2)13-14(10,11-3)12-4/h5H,1-4H3,(H,8,9)/b6-5-
InchiKey: KRTSDMXIXPKRQR-WAYWQWQTSA-N
Formula: C7H14NO5P
SMILES: CNC(=O)C=C(C)OP(=O)(OC)OC
Mol. weight [g/mol]: 223.16
CAS: 919-44-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.59		Crippen Method
logp	1.054		Crippen Method
mcvol	160.680	ml/mol	McGowan Method
rinpol	1673.00		NIST Webbook
rinpol	1684.00		NIST Webbook
rinpol	1690.00		NIST Webbook
rinpol	1645.00		NIST Webbook
rinpol	1707.00		NIST Webbook
rinpol	1675.00		NIST Webbook
rinpol	1660.00		NIST Webbook
rinpol	1679.00		NIST Webbook
rinpol	1660.00		NIST Webbook

Sources

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=C919448&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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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