

Tris(1-(2-methyl)aziridinyl)phosphine oxide

Other names:	Aziridine, 1,1',1''-phosphinylidynetris[2-methyl- C 3172 EMT 50,003 ENT 50,003 Metapoxide Metepa Methaphoxide Methyl aphoxide MAPO N,N',N''-Tris(1-methylethylene)phosphoramide Phosphine oxide, tris(2-methyl-1-aziridinyl)- Phosphine oxide, tris(1-(2-methyl)aziridinyl)- Trimethylaziridinylphosphine oxide Tris(methylaziridinyl)phosphine oxide Tris(1-methylethylene)phosphoric triamide Tris(1,2-propylene)phosphoramide Tris(2-methyl-1-aziridinyl)phosphine oxide Tris(2-methylaziridin-1-yl)phosphine oxide Tris(2-methylaziridinyl)phosphine oxide 1,1',1''-Phosphinylidynetris(2-methyl)aziridine Metapa NSC 54054 TEPA
Inchi:	InChI=1S/C9H18N3OP/c1-7-4-10(7)14(13,11-5-8(11)2)12-6-9(12)3/h7-9H,4-6H2,1-3H3
InchiKey:	AVUYXHYHTTVPRX-UHFFFAOYSA-N
Formula:	C9H18N3OP
SMILES:	CC1CN1P(=O)(N1CC1C)N1CC1C
Mol. weight [g/mol]:	215.23
CAS:	57-39-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.58		Crippen Method
logp	1.207		Crippen Method
mcvol	161.360	ml/mol	McGowan Method

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=C57396&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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