

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

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | Aziridine, 1,1',1''-phosphinylidynetris[2-methyl-C 3172<br>EMT 50,003<br>ENT 50,003<br>Metapoxide<br>Metepa<br>Methaphoxide<br>Methyl aphoxide<br>MAPO<br>N,N',N''-Tris(1-methylethylene)phosphoramid<br>Phosphine oxide, tris(2-methyl-1-aziridinyl)-<br>Phosphine oxide, tris(1-(2-methyl)aziridinyl)-<br>Trimethylaziridinylphosphine oxide<br>Tris(methylaziridinyl)phosphine oxide<br>Tris(1-methylethylene)phosphoric triamide<br>Tris(1,2-propylene)phosphoramid<br>Tris(2-methyl-1-aziridinyl)phosphine oxide<br>Tris(2-methylaziridin-1-yl)phosphine oxide<br>Tris(2-methylaziridinyl)phosphine oxide<br>1,1',1''-Phosphinylidynetris(2-methyl)aziridine<br>Metapa<br>NSC 54054<br>TEPA |
| <b>Inchi:</b>               | 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   |
| <b>InchiKey:</b>            | AVUYXHYHTTVPRX-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C9H18N3OP  |
| <b>SMILES:</b>              | CC1CN1P(=O)(N1CC1C)N1CC1C  |
| <b>Mol. weight [g/mol]:</b> | 215.23   |
| <b>CAS:</b>                 | 57-39-6  |

## Physical Properties

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

# Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                               |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                       |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                   |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C57396&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C57396&amp;Units=SI</a> |

# Legend

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

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