

# Paramethadione

|                      |                                                                                                                                                                                                                                       |
|----------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | 2,4-Oxazolidinedione, 5-ethyl-3,5-dimethyl-Paradione<br>Parametadione<br>A 348<br>3,5-Dimethyl-5-ethyloxazolidine-2,4-dione<br>5-Ethyl-3,5-dimethyloxazolidine-2,4-dione<br>Isoethadione<br>5-Ethyl-3,5-dimethyl-2,4-oxazolidinedione |
| Inchi:               | InChI=1S/C7H11NO3/c1-4-7(2)5(9)8(3)6(10)11-7/h4H2,1-3H3                                                                                                                                                                               |
| InchiKey:            | VQASKUSHBVDKGU-UHFFFAOYSA-N                                                                                                                                                                                                           |
| Formula:             | C7H11NO3                                                                                                                                                                                                                              |
| SMILES:              | <chem>CCC1(C)OC(=O)N(C)C1=O</chem>                                                                                                                                                                                                    |
| Mol. weight [g/mol]: | 157.17                                                                                                                                                                                                                                |
| CAS:                 | 115-67-3                                                                                                                                                                                                                              |

## Physical Properties

| Property code | Value         | Unit   | Source         |
|---------------|---------------|--------|----------------|
| log10ws       | -0.94         |        | Crippen Method |
| logp          | 0.764         |        | Crippen Method |
| mcvol         | 117.620       | ml/mol | McGowan Method |
| rinpol        | 1120.00       |        | NIST Webbook   |
| tf            | 334.45 ± 0.50 | K      | NIST Webbook   |

## Sources

|                 |                                                                                                                                           |
|-----------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C115673&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C115673&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     |
| <b>rinpol:</b>  | Non-polar retention indices         |
| <b>tf:</b>      | Normal melting (fusion) point       |

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