

# 2,4-Imidazolidinedione, 1,3-diethyl-5,5-diphenyl-

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | Phenytoin perethylated   |
| <b>Inchi:</b>               | InChI=1S/C19H20N2O2/c1-3-20-17(22)19(21(4-2)18(20)23,15-11-7-5-8-12-15)16-13-9-6 |
| <b>InchiKey:</b>            | MBPAFXVXFARGCF-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C19H20N2O2   |
| <b>SMILES:</b>              | CCN1C(=O)N(CC)C(c2ccccc2)(c2ccccc2)C1=O  |
| <b>Mol. weight [g/mol]:</b> | 308.37   |
| <b>CAS:</b>                 | 54964-77-1   |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -3.82   |        | Crippen Method |
| logp          | 3.234   |        | Crippen Method |
| mcvol         | 243.290 | ml/mol | McGowan Method |
| rinpol        | 2295.00 |        | NIST Webbook   |
| rinpol        | 2295.00 |        | NIST Webbook   |

## Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C54964771&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C54964771&amp;Units=SI</a> |
| <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>                         |

## 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         |

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