

2,4-Imidazolidinedione, 3-methyl-

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| Other names: | Hydantoin, 3-methyl- 3-Methylhydantoin 2,4-Imidazolidinedione, 4-methyl- |
| Inchi: | InChI=1S/C4H6N2O2/c1-6-3(7)2-5-4(6)8/h2H2,1H3,(H,5,8) |
| InchiKey: | MZQQHYDUINOMDG-UHFFFAOYSA-N |
| Formula: | C4H6N2O2 |
| SMILES: | CN1C(=O)CNC1=O |
| Mol. weight [g/mol]: | 114.10 |
| CAS: | 6843-45-4 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|-------------|--------|----------------|
| ie | 9.70 | eV | NIST Webbook |
| ie | 9.87 ± 0.05 | eV | NIST Webbook |
| log10ws | 0.32 | | Crippen Method |
| logp | -0.832 | | Crippen Method |
| mcvol | 79.460 | 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=C6843454&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

Legend

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

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<https://www.cheméo.com/cid/50-054-6/2-4-Imidazolidinedione-3-methyl.pdf>

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