

# 2,4-Imidazolidinedione, 3-ethyl-5-phenyl-

|                      |                                                                                                                                                                                                                                                                |
|----------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | 2,4-Imidazolidinedione, 3-ethyl-5-phenyl-<br>Hydantoin, 3-ethyl-5-phenyl-<br>Accenon<br>AC-695<br>Peganone<br>3-Ethyl-5-phenylhydantoin<br>1-Ethyl-2,5-dioxo-4-phenylimidazolidine<br>3-Ethyl-5-phenylimidazolidin-2,4-dione<br>Pegoanone<br>(. +/-.)-Ethotoin |
| Inchi:               | InChI=1S/C11H12N2O2/c1-2-13-10(14)9(12-11(13)15)8-6-4-3-5-7-8/h3-7,9H,2H2,1H3,(H                                                                                                                                                                               |
| InchiKey:            | SZQIFWWUIBRPBZ-UHFFFAOYSA-N                                                                                                                                                                                                                                    |
| Formula:             | C11H12N2O2                                                                                                                                                                                                                                                     |
| SMILES:              | CCN1C(=O)NC(c2ccccc2)C1=O                                                                                                                                                                                                                                      |
| Mol. weight [g/mol]: | 204.23                                                                                                                                                                                                                                                         |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| logp          | 1.299   |        | Crippen Method |
| mcvol         | 154.330 | ml/mol | McGowan Method |
| rinpol        | 1790.00 |        | NIST Webbook   |
| rinpol        | 1800.00 |        | NIST Webbook   |
| rinpol        | 1800.00 |        | NIST Webbook   |
| rinpol        | 1790.00 |        | NIST Webbook   |

## Sources

|                           |                                                                                                                                         |
|---------------------------|-----------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method:           | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                       |
| Cheméo Relay (1.0):       |                                                                                                                                         |
| Cheméo Relay (1.0, beta): |                                                                                                                                         |
| NIST Webbook:             | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C86351&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C86351&amp;Units=SI</a> |
| McGowan Method:           | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                   |
| Crippen Method:           | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                               |

# Legend

|                |                                     |
|----------------|-------------------------------------|
| <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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