

# 2-Furamide, n-benzimidazole-2-yl-

|                      |                                                                                  |
|----------------------|----------------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C12H9N3O2/c16-11(10-6-3-7-17-10)15-12-13-8-4-1-2-5-9(8)14-12/h1-7H,(H2, |
| InchiKey:            | ZVRZJITVEDLUKY-UHFFFAOYSA-N                                                      |
| Formula:             | C12H9N3O2                                                                        |
| SMILES:              | O=C(Nc1nc2ccccc2[nH]1)c1ccco1                                                    |
| Mol. weight [g/mol]: | 227.22                                                                           |
| CAS:                 | 21694-48-4                                                                       |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -7.97   |        | Crippen Method |
| logp          | 1.926   |        | Crippen Method |
| mcvol         | 158.940 | ml/mol | McGowan Method |

## Sources

|                 |                                                                                                                                               |
|-----------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| 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=C21694484&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C21694484&amp;Units=SI</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

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

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