

# Nitrofurantoin

**Other names:**

- 1-(5-Nitro-2-furfurylidenamino)hydantoin
- 1-(5-Nitro-2-furfurylideneamino)hydantoin
- 1-[(5-Nitrofurfurylidene)amino]hydantoin
- 2,4-Imidazolidinedione, 1-[[5-nitro-2-furanyl)methylene]amino]-
- 5-Nitrofurantoin
- 5-Nitrofurantoin dorn
- Benkfuran
- Berkfurin
- Chemiofuran
- Cyantoin
- Cystit
- Dantafur
- Fua Med
- Fur-ren
- Furachel
- Furadantin
- Furadantine
- Furadantine MC
- Furadantoin
- Furadoine
- Furadonin
- Furadonine
- Furadontin
- Furalan
- Furaloid
- Furantoin
- Furatoin
- Furina
- Furobactina
- Hydantoin, 1-[(5-nitrofurfurylidene)amino]-
- Hydantoin, n-(5-nitro-2-furfurylidene)-1-amino-
- Ituran
- Macpac
- Macrobid
- Macrofantin
- N-(5-Nitro-2-furfurylidene)-1-aminohydantoin
- N-(5-Nitro-2-furfurylidene)-1-aminohydantoina
- N-(5-Nitrofurfurylidene)-1-aminohydantoin
- N-Toin
- NCI-C55196

NSC-2107  
Nierofu  
Nifurantin  
Nitoin  
Nitrex  
Nitrofuradantin  
Novofuran  
Orafuran  
Parfuran  
Trantoin  
USAF EA-2  
Urantoin  
Urizept  
Uro-Tablinen  
Urodin  
Urofurin  
Urolong  
Welfurin  
Zoofurin

**Inchi:** InChI=1S/C8H6N4O5/c13-6-4-11(8(14)10-6)9-3-5-1-2-7(17-5)12(15)16/h1-3H,4H2,(H,10)  
**InchiKey:** NXFQHRVNIOXGAQ-UHFFFAOYSA-N  
**Formula:** C8H6N4O5  
**SMILES:** O=C1CN(N=Cc2ccc([N+](=O)[O-])o2)C(=O)N1  
**Mol. weight [g/mol]:** 238.16  
**CAS:** 67-20-9

## Physical Properties

| Property code | Value   | Unit   | Source                      |
|---------------|---------|--------|-----------------------------|
| log10ws       | -3.38   |        | Estimated Solubility Method |
| logp          | 0.073   |        | Crippen Method              |
| mcvol         | 145.330 | ml/mol | McGowan Method              |

## Sources

**Estimated Solubility Method:** [http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl\\_file/ci034243xsi20040112\\_053635.txt](http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C67209&Units=SI>

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

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

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