

# 4-NITROBENZOFUROXAN

|                      |                                                                                                                             |
|----------------------|-----------------------------------------------------------------------------------------------------------------------------|
| Other names:         | 4-Nitrobenzofuroxan<br>B2789<br>Nitrobenzofuroxan<br>2,1,3-Benzoxadiazole, 4-nitro-, 1-oxide<br>4-Nitrobenzofuroxan-1-oxide |
| Inchi:               | InChI=1S/C6H3N3O4/c10-8(11)4-2-1-3-5-6(4)7-13-9(5)12/h1-3H                                                                  |
| InchiKey:            | XUCKCDGEIRMZPM-UHFFFAOYSA-N                                                                                                 |
| Formula:             | C6H3N3O4                                                                                                                    |
| SMILES:              | O=[N+]([O-])c1cccc2c1no[n+](O-)                                                                                             |
| Mol. weight [g/mol]: | 181.11                                                                                                                      |

## Physical Properties

| Property code | Value   | Unit   | Source             |
|---------------|---------|--------|--------------------|
| hf            | 294.47  | kJ/mol | Cheméo Relay (1.0) |
| ie            | 9.65    | eV     | Cheméo Relay (1.0) |
| log10ws       | -2.57   |        | Cheméo Relay (1.0) |
| logp          | 0.369   |        | Crippen Method     |
| mcvol         | 105.600 | ml/mol | McGowan Method     |
| tf            | 395.91  | K      | Cheméo Relay (1.0) |

## Sources

|                           |                                                                                                                                               |
|---------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method:           | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                     |
| 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=C18771852&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C18771852&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>                         |

## Legend

|                 |                                              |
|-----------------|----------------------------------------------|
| <b>hf:</b>      | Enthalpy of formation at standard conditions |
| <b>ie:</b>      | Ionization energy                            |
| <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>tf:</b>      | Normal melting (fusion) point                |

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