

# Piperidine, 1-(2,4-dinitrophenyl)-

|                             |                                                                                  |
|-----------------------------|----------------------------------------------------------------------------------|
| <b>Other names:</b>         | 1-(2,4-dinitrophenyl)piperidine                                                  |
| <b>Inchi:</b>               | InChI=1S/C11H13N3O4/c15-13(16)9-4-5-10(11(8-9)14(17)18)12-6-2-1-3-7-12/h4-5,8H,1 |
| <b>InchiKey:</b>            | MPGYUYKSTWTQFS-UHFFFAOYSA-N                                                      |
| <b>Formula:</b>             | C11H13N3O4                                                                       |
| <b>SMILES:</b>              | O=[N+]([O-])c1ccc(N2CCCCC2)c([N+](=O)[O-])c1                                     |
| <b>Mol. weight [g/mol]:</b> | 251.24                                                                           |
| <b>CAS:</b>                 | 839-93-0                                                                         |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -3.83   |        | Crippen Method |
| logp          | 2.493   |        | Crippen Method |
| mcvol         | 176.050 | ml/mol | McGowan Method |

## Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C839930&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C839930&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |

## Legend

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

Latest version available from:

<https://www.chemeo.com/cid/119-855-1/Piperidine-1-2-4-dinitrophenyl.pdf>

Generated by Cheméo on 2024-04-27 19:54:58.950454872 +0000 UTC m=+16536947.871032182.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.