

1H-Imidazole, 4-methyl-5-nitro-

| | |
|-----------------------------|---|
| Other names: | Imidazole, 4-methyl-5-nitro- 4-Methyl-5-nitroimidazole 5-Methyl-4-nitroimidazole Imidazole, 5-methyl-4-nitro- 4-Methyl-5-nitro-1H-imidazole Imidazole, 4(or 5)-methyl-5(or 4)-nitro- |
| Inchi: | InChI=1S/C4H5N3O2/c1-3-4(7(8)9)6-2-5-3/h2H,1H3,(H,5,6) |
| InchiKey: | WSYOWIMKNNMEMZ-UHFFFAOYSA-N |
| Formula: | C4H5N3O2 |
| SMILES: | <chem>Cc1nc[nH]c1[N+](=O)[O-]</chem> |
| Mol. weight [g/mol]: | 127.10 |
| CAS: | 14003-66-8 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|--------|--------|----------------|
| log10ws | -1.58 | | Crippen Method |
| logp | 0.144 | | Crippen Method |
| mcvol | 85.140 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C14003668&Units=SI |

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/30-872-0/1H-Imidazole-4-methyl-5-nitro.pdf>

Generated by Cheméo on 2024-04-17 03:01:36.222102402 +0000 UTC m=+15612145.142679717.

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