

# 1-METHYL-3-NITROPYRAZOLE

**Inchi:** InChI=1S/C4H5N3O2/c1-6-3-2-4(5-6)7(8)9/h2-3H,1H3  
**InchiKey:** KLAQNTBUXCCZHC-UHFFFAOYSA-N  
**Formula:** C4H5N3O2  
**SMILES:** Cn1ccc([N+](=O)[O-])n1  
**Mol. weight [g/mol]:** 127.10

## Physical Properties

| Property code | Value  | Unit   | Source         |
|---------------|--------|--------|----------------|
| affp          | 847.60 | kJ/mol | NIST Webbook   |
| basg          | 815.70 | kJ/mol | NIST Webbook   |
| logp          | 0.328  |        | Crippen Method |
| mcvol         | 85.140 | ml/mol | McGowan Method |

## Sources

Cheméo Relay (1.0, beta):

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C54210321&Units=SI>

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

Cheméo Relay (1.0):

## Legend

**affp:** Proton affinity  
**basg:** Gas basicity  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume

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