

Pyrazole, 3-nitro-

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|-----------------------------|---|
| Other names: | 3-Nitro-1H-pyrazole Djw 94 3(5)-nitropyrazole |
| Inchi: | InChI=1S/C3H3N3O2/c7-6(8)3-1-2-4-5-3/h1-2H,(H,4,5) |
| InchiKey: | MZRUFMBFIKGOAL-UHFFFAOYSA-N |
| Formula: | C3H3N3O2 |
| SMILES: | O=[N+](O-)c1cc[nH]n1 |
| Mol. weight [g/mol]: | 113.07 |
| CAS: | 26621-44-3 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|--------|--------|----------------|
| affp | 820.80 | kJ/mol | NIST Webbook |
| basg | 789.00 | kJ/mol | NIST Webbook |
| log10ws | -1.11 | | Crippen Method |
| logp | -0.164 | | Crippen Method |
| mcvol | 71.050 | 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=C26621443&Units=SI |

Legend

| | |
|-----------------|-------------------------------------|
| affp: | Proton affinity |
| basg: | Gas basicity |
| 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/122-189-7/Pyrazole-3-nitro.pdf>

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