

6-Methyl-5-nitroquinoline

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| Other names: | 5-Nitro-6-methylquinoline Quinoline, 6-methyl-5-nitro- |
| Inchi: | InChI=1S/C10H8N2O2/c1-7-4-5-9-8(3-2-6-11-9)10(7)12(13)14/h2-6H,1H3 |
| InchiKey: | CENBTULRDDPOGR-UHFFFAOYSA-N |
| Formula: | C10H8N2O2 |
| SMILES: | <chem>Cc1ccc2ncccc2c1[N+](=O)[O-]</chem> |
| Mol. weight [g/mol]: | 188.18 |
| CAS: | 23141-61-9 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -4.17 | | Crippen Method |
| logp | 2.451 | | Crippen Method |
| mcvol | 135.940 | ml/mol | McGowan Method |
| rinpol | 277.76 | | NIST Webbook |
| rinpol | 271.61 | | NIST Webbook |
| rinpol | 277.29 | | NIST Webbook |
| rinpol | 275.97 | | NIST Webbook |

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=C23141619&Units=SI |

Legend

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

rinpol: Non-polar retention indices

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<https://www.chemeo.com/cid/16-024-7/6-Methyl-5-nitroquinoline.pdf>

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