

1-Methyl-4-nitro-5-(o-acetamidophenylsulfinyl)imidazole

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|-----------------------------|--|
| Inchi: | InChI=1S/C12H12N4O4S/c1-8(17)14-9-5-3-4-6-10(9)21(20)12-11(16(18)19)13-7-15(12)2 |
| InchiKey: | UACSPGWZIHVVIT-UHFFFAOYSA-N |
| Formula: | C12H12N4O4S |
| SMILES: | CC(=O)Nc1cccc1S(=O)c1c([N+](=O)[O-])ncn1C |
| Mol. weight [g/mol]: | 308.31 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -4.55 | | Crippen Method |
| logp | 1.453 | | Crippen Method |
| mcvol | 207.870 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.cheméo.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=B6008345&Units=SI |

Legend

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

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