

6-Methyl-4-oxo-1,2,3a,7-tetrazaindene

| | |
|-----------------------------|--|
| Inchi: | InChI=1S/C6H6N4O/c1-4-2-5(11)10-3-7-9-6(10)8-4/h2-3H,1H3,(H,8,9) |
| InchiKey: | NWZKLXIFHRN XKJ-UHFFFAOYSA-N |
| Formula: | C6H6N4O |
| SMILES: | Cc1cc(=O)n2cn[nH]c2n1 |
| Mol. weight [g/mol]: | 150.14 |
| CAS: | 41081-90-7 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -1.08 | | Crippen Method |
| logp | -0.756 | | Crippen Method |
| mcvol | 102.270 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C41081907&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

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.chemeo.com/cid/98-612-4/6-Methyl-4-oxo-1-2-3a-7-tetrazaindene.pdf>

Generated by Cheméo on 2024-05-02 03:47:10.597657909 +0000 UTC m=+16910879.518235225.

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