

4(1H)-Pyrimidinone, 6-hydroxy-

| | |
|-----------------------------|---|
| Other names: | 4(3H)-Pyrimidinone, 6-hydroxy- 4,6-Dihydroxypyrimidine 4,6-Pyrimidinediol 6-Hydroxy-4(1H)-pyrimidinone 6-hydroxy-1H-pyrimidin-4-one |
| Inchi: | InChI=1S/C4H4N2O2/c7-3-1-4(8)6-2-5-3/h1-2H,(H2,5,6,7,8) |
| InchiKey: | DUFGYCAXVIUXIP-UHFFFAOYSA-N |
| Formula: | C4H4N2O2 |
| SMILES: | Oc1cc(O)ncn1 |
| Mol. weight [g/mol]: | 112.09 |
| CAS: | 1193-24-4 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|--------|--------|----------------|
| log10ws | -0.10 | | Crippen Method |
| logp | -0.112 | | Crippen Method |
| mcvol | 75.160 | 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=C1193244&Units=SI |

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.cheméo.com/cid/13-529-0/4-1H-Pyrimidinone-6-hydroxy.pdf>

Generated by Cheméo on 2024-04-17 03:52:23.205639347 +0000 UTC m=+15615192.126216711.

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