

Lumazine

| | |
|-----------------------------|---|
| Other names: | 2,4(1H,3H)-Pteridinedione 2,4(3H,8H)-Pteridinedione 2,4-Dihydroxypteridine 2,4-Pteridinediol Lumazin Pteridinedione, 2,4(1h,3h)- pteridine-2,4-diol monohydrate |
| Inchi: | InChI=1S/C6H4N4O2/c11-5-3-4(8-2-1-7-3)9-6(12)10-5/h1-2H,(H2,8,9,10,11,12) |
| InchiKey: | UYEUUXMDVNYCAM-UHFFFAOYSA-N |
| Formula: | C6H4N4O2 |
| SMILES: | O=c1[nH]c(=O)c2nccnc2[nH]1 |
| Mol. weight [g/mol]: | 164.12 |
| CAS: | 487-21-8 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| ie | 9.20 | eV | NIST Webbook |
| log10ws | -0.09 | | Crippen Method |
| logp | -1.957 | | Crippen Method |
| mvol | 103.840 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C487218&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |

Legend

ie: Ionization energy

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/37-507-8/Lumazine.pdf>

Generated by Cheméo on 2024-04-29 05:21:59.016920567 +0000 UTC m=+16657367.937497880.

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