

3,4-Pyridinedimethanol, 5-hydroxy-6-methyl-

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| Other names: | 2-Methyl-3-hydroxy-4,5-bis(hydroxymethyl)pyridine 2-Methyl-3-hydroxy-4,5-di(hydroxymethyl)pyridine 2-Methyl-3-hydroxy-4,5-dihydroxymethyl-pyridin 2-Methyl-4,5-bis(hydroxymethyl)-3-hydroxypyridine 2-Picoline-4,5-dimethanol, 3-hydroxy- 3-Hydroxy-4,5-dimethylol-«alpha»-picoline 4,5-bis(hydroxymethyl)-2-methylpyridin-3-ol 5-hydroxy-6-methyl-3,4-pyridinedimethanol Adermin Adermine Bezatin Gravidox Hydoxin Pirivitol Pridoxine Pyridoxin Pyridoxine Pyridoxinum Pyridoxol |
| Inchi: | InChI=1S/C8H11NO3/c1-5-8(12)7(4-11)6(3-10)2-9-5/h2,10-12H,3-4H2,1H3 |
| InchiKey: | LXNHXLLTXMVWPM-UHFFFAOYSA-N |
| Formula: | C8H11NO3 |
| SMILES: | Cc1ncc(CO)c(CO)c1O |
| Mol. weight [g/mol]: | 169.18 |
| CAS: | 65-23-6 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|--|
| hfus | 31.15 | kJ/mol | Antisolvent Precipitation of Vitamin B6: A Thermodynamic Study |
| log10ws | -1.55 | | Crippen Method |
| logp | 0.080 | | Crippen Method |
| mcvol | 127.410 | ml/mol | McGowan Method |
| ss | 271.77 | J/molxK | NIST Webbook |
| ss | 278.59 | J/molxK | NIST Webbook |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|--------------|
| cps | 237.40 | J/mol×K | 300.00 | NIST Webbook |
| cps | 244.46 | J/mol×K | 298.15 | NIST Webbook |

Sources

| | |
|--|--|
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Antisolvent Precipitation of Vitamin B6: A Thermodynamic Study: McGowan Method: | https://www.doi.org/10.1021/je200853g http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C65236&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

Legend

| | |
|-----------------|--|
| cps: | Solid phase heat capacity |
| hfus: | Enthalpy of fusion at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| ss: | Solid phase molar entropy at standard conditions |

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