

7H-imidazo[4,5-d]-v-triazin-4-one, 6-methyl-

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|-----------------------------|--|
| Inchi: | InChI=1S/C5H5N5O/c1-2-6-3-4(7-2)8-10-9-5(3)11/h1H3,(H2,6,7,8,9,11) |
| InchiKey: | KWGOKRBOKHHRDP-UHFFFAOYSA-N |
| Formula: | C5H5N5O |
| SMILES: | Cc1nc2c(O)nnnc2[nH]1 |
| Mol. weight [g/mol]: | 151.13 |
| CAS: | 94190-03-1 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|--------|--------|----------------|
| log10ws | -1.58 | | Crippen Method |
| logp | -0.720 | | Crippen Method |
| mcvol | 98.160 | 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=C94190031&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 |

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