Pyrimidine, 6-oxo-5-acetyl-4-hydroxy-1,6-dihydro-

Other names: 6-Hydroxy-5-acetyl-4-oxo-1,6-dihydropyrimidine
Inchi: InChI=1S/C6H6N2O3/c1-3(9)4-5(10)7-2-8-6(4)11/h2H,1H3,(H2,7,8,10,11)
InchiKey: PYJZBCIQPVBBPY-UHFFFAOYSA-N
Formula: C6H6N2O3
SMILES: CC(=O)c1c(O)nc[nH]c1=O
Mol. weight [g/mol]: 154.12
CAS: 98792-81-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.09		Crippen Method
logp	-0.804		Crippen Method
mcvol	104.910	ml/mol	McGowan Method

Sources

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=C98792815&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume