2-Pyrimidinecarbamonitrile, 4-amino-6-hydroxy- (keto form)

Inchi: InChI=1S/C5H5N5O/c6-2-8-5-9-3(7)1-4(11)10-5/h1H,(H4,7,8,9,10,11)
InchiKey: JQZJMILBKZUKLV-UHFFFAOYSA-N
Formula: C5H5N5O
SMILES: N#CN=c1nc(O)cc(N)[nH]1
Mol. weight [g/mol]: 151.13
CAS: 6112-71-6

Physical Properties

Property code	Value	Unit	Source
log10ws	0.34		Crippen Method
logp	-1.403		Crippen Method
mcvol	104.720	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=C6112716&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