2-Pyrimidinecarbamonitrile, 1,6-dihydro-4-methyl-6-oxo-

Inchi: InChI=1S/C6H6N4O/c1-4-2-5(11)10-6(9-4)8-3-7/h2H,1H3,(H2,8,9,10,11)
InchiKey: WGBRHUINONWPFT-UHFFFAOYSA-N
Formula: C6H6N4O
SMILES: Cc1cc(O)nc(=NC#N)[nH]1
Mol. weight [g/mol]: 150.14
CAS: 7152-19-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.50		Crippen Method
logp	-0.676		Crippen Method
mcvol	108.830	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7152194&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

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