2-AMINO-6-METHYL-4-PYRIMIDINOL

Other names:	2-Amino-4-oxo-6-methylpyrimidine
	2-Amino-6-methyl-4-pyrimidinol
	2-Amino-6-methylpyrimidin-4-ol
	4(1H)-Pyrimidinone, 2-amino-6-methyl-
	4-Methylisocytosine
	4-Pyrimidinol, 2-amino-6-methyl-
	6-Methylisocytosine
	Mecytosine
	NSC 13145
	NSC 23662
	NSC 41833
	NSC 7893
	Pyrimidine, 2-amino-4-hydroxy-6-methyl- (keto form)
	Superacil
	Superacyl
Inchi:	InChI=1S/C5H7N3O/c1-3-2-4(9)8-5(6)7-3/h2H,1H3,(H3,6,7,8,9)
InchiKey:	KWXIPEYKZKIAKR-UHFFFAOYSA-N
Formula:	C5H7N3O
SMILES:	Cc1cc(O)nc(N)n1
Mol. weight [g/mol]:	125.13

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.70		Cheméo Relay (1.0)
logp	0.073		Crippen Method
mcvol	93.360	ml/mol	McGowan Method
tb	533.91	K	Cheméo Relay (1.0)
tf	512.48	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3977295&Units=SI

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point