Pyrimidine, 4,6-dimethyl-

Other names: 4,6-Dimethylpyrimidine
Inchi: InChI=1S/C6H8N2/c1-5-3-6(2)8-4-7-5/h3-4H,1-2H3
InchiKey: LSBIUXKNVUBKRI-UHFFFAOYSA-N
Formula: C6H8N2
SMILES: Cc1cc(C)ncn1
Mol. weight [g/mol]: 108.14
CAS: 1558-17-4

Physical Properties

Property code	Value	Unit	Source
affp	928.00 ± 1.00	kJ/mol	NIST Webbook
log10ws	-1.95		Crippen Method
logp	1.093		Crippen Method
mcvol	91.600	ml/mol	McGowan Method
ripol	1381.00		NIST Webbook
ripol	1363.00		NIST Webbook
ripol	1363.00		NIST Webbook
tb	427.20	K	NIST Webbook
tb	432.00 ± 6.00	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	432.70	K	101.00	NIST Webbook

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=C1558174&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure