Pyrimidine, 4-methyl-

Other names: 4-Methylpyrimidine
Inchi: InChI=1S/C5H6N2/c1-5-2-3-6-4-7-5/h2-4H,1H3
InchiKey: LVILGAOSPDLNRM-UHFFFAOYSA-N
Formula: C5H6N2
SMILES: Cc1ccncn1
Mol. weight [g/mol]: 94.11
CAS: 3438-46-8

Physical Properties

Property code	Value	Unit	Source
hvap	44.20 ± 2.40	kJ/mol	NIST Webbook
log10ws	-1.48		Crippen Method
logp	0.785		Crippen Method
mcvol	77.510	ml/mol	McGowan Method
rinpol	827.00		NIST Webbook
rinpol	853.00		NIST Webbook
rinpol	827.00		NIST Webbook
rinpol	819.00		NIST Webbook
rinpol	853.00		NIST Webbook
ripol	1328.00		NIST Webbook
tb	415.20	K	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=C3438468&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature