

Pyrimidine, 4-methyl-

Other names:	4-Methylpyrimidine
Inchi:	InChI=1S/C5H6N2/c1-5-2-3-6-4-7-5/h2-4H,1H3
InchiKey:	LVILGAOSPDNLNRM-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
mcpol	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/ci9903071

Legend

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
ri_{npol}:	Non-polar retention indices
ri_{pol}:	Polar retention indices
tb:	Normal Boiling Point Temperature

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