

Pyrimidine, 5-methyl-

Other names:	5-Methylpyrimidine
Inchi:	InChI=1S/C5H6N2/c1-5-2-6-4-7-3-5/h2-4H,1H3
InchiKey:	TWGNOYAGHYUFFR-UHFFFAOYSA-N
Formula:	C5H6N2
SMILES:	Cc1cncnc1
Mol. weight [g/mol]:	94.11
CAS:	2036-41-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.48		Crippen Method
logp	0.785		Crippen Method
mcvol	77.510	ml/mol	McGowan Method
rinpol	864.00		NIST Webbook
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rinpol	864.00		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=C2036411&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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