

Pyrimidine, 4,5-dimethyl-

Other names:	4,5-Dimethylpyrimidine
Inchi:	InChI=1S/C6H8N2/c1-5-3-7-4-8-6(5)2/h3-4H,1-2H3
InchiKey:	XPCYMUBTCGGWOH-UHFFFAOYSA-N
Formula:	C6H8N2
SMILES:	Cc1cncnc1C
Mol. weight [g/mol]:	108.14
CAS:	694-81-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.95		Crippen Method
logp	1.093		Crippen Method
mcvol	91.600	ml/mol	McGowan Method
ripol	1395.00		NIST Webbook
ripol	1395.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C694815&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Polar retention indices

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