

Pyrimido [5,4-e]-as-triazine, 1,2-dihydro-

Inchi:	InChI=1S/C5H5N5/c1-4-5(8-2-6-1)10-9-3-7-4/h1-3H,(H,7,9)(H,6,8,10)
InchiKey:	KRXOCAKGVQYFOA-UHFFFAOYSA-N
Formula:	C5H5N5
SMILES:	C1=Nc2cncnc2NN1
Mol. weight [g/mol]:	135.13
CAS:	19801-79-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.31		Crippen Method
logp	0.066		Crippen Method
mcvol	92.290	ml/mol	McGowan Method

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=C19801797&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/80-837-4/Pyrimido-5-4-e-as-triazine-1-2-dihydro.pdf>

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