

Pyrimido[5,4-e]-as-triazin-5[6h]-one, 1,2-dihydro-

Inchi:	InChI=1S/C5H5N5O/c11-5-3-4(7-1-8-5)10-9-2-6-3/h1-2H,(H,6,9)(H2,7,8,10,11)
InchiKey:	MCLXITSMNGGMMMA-UHFFFAOYSA-N
Formula:	C5H5N5O
SMILES:	Oc1ncnc2c1N=CN2
Mol. weight [g/mol]:	151.13

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.86		Crippen Method
logp	-0.228		Crippen Method
mcvol	98.160	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=B6008723&Units=SI

Legend

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

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