

5-Methyl-7-oxo-1,2,3a,4-tetrazaindene

Inchi:	InChI=1S/C6H6N4O/c1-4-2-5(11)6-7-3-8-10(6)9-4/h2-3,9H,1H3
InchiKey:	KWIPAFVAXBZRCE-UHFFFAOYSA-N
Formula:	C6H6N4O
SMILES:	Cc1cc(=O)c2ncnn2[nH]1
Mol. weight [g/mol]:	150.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.08		Crippen Method
logp	-0.756		Crippen Method
mcvol	102.270	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6002146&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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