

4-Methyl-6-oxo-1,2,3a,7-tetrazaindene

Inchi:	InChI=1S/C6H6N4O/c1-4-2-5(11)8-6-9-7-3-10(4)6/h2-3H,1H3,(H,8,9,11)
InchiKey:	KNDVOXYNXZHWSJ-UHFFFAOYSA-N
Formula:	C6H6N4O
SMILES:	Cc1cc(O)nc2nncn12
Mol. weight [g/mol]:	150.14
CAS:	69924-53-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.75		Crippen Method
logp	0.138		Crippen Method
mcvol	102.270	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C69924534&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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