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

Inchi:	InChI=1S/C6H6N4O/c1-4-2-5(11)9-6-7-3-8-10(4)6/h2-3H,1H3,(H,7,8,9,11)
InchiKey:	BOPVGQUDDIEQAO-UHFFFAOYSA-N
Formula:	C6H6N4O
SMILES:	Cc1cc(=O)[nH]c2ncnn12
Mol. weight [g/mol]:	150.14
CAS:	5217-59-4

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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C5217594&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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