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

Inchi: InChI=1S/C6H6N4O/c1-4-2-5(11)10-6(9-4)7-3-8-10/h2-3H,1H3,(H,7,8,9)
InchiKey: INVVMIXYILXINW-UHFFFAOYSA-N
Formula: C6H6N4O
SMILES: Cc1cc(=O)n2[nH]cnc2n1
Mol. weight [g/mol]: 150.14
CAS: 35523-67-2

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: 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=C35523672&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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