

2,6-Diamino-4-oxo-1,3,3a,7-tetrazaindene mono-hydrochloride

Inchi:	InChI=1S/C5H6N6O/c6-2-1-3(12)11-5(8-2)9-4(7)10-11/h1H,6H2,(H3,7,8,9,10)
InchiKey:	PBXXNZHAPNXEJP-UHFFFAOYSA-N
Formula:	C5H6N6O
SMILES:	<chem>Nc1nc2[nH]c(N)cc(=O)n2n1</chem>
Mol. weight [g/mol]:	166.14

Physical Properties

Property code	Value	Unit	Source
log10ws	0.13		Crippen Method
logp	-1.900		Crippen Method
mcvol	108.140	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6002139&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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