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: Nc1nc2[nH]c(N)cc(=O)n2n1
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/ci990307l
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