N-[4-(6-methyl)-1,3,3a,7-tetrazaindenyl]-ethylened hydrochloride

Inchi: InChI=1S/C8H12N6/c1-6-4-7(10-3-2-9)14-8(13-6)11-5-12-14/h4-5,10H,2-3,9H2,1H3

InchiKey: DROUECPSPOUPDI-UHFFFAOYSA-N

Formula: C8H12N6

SMILES: Cc1cc(NCCN)n2ncnc2n1

Mol. weight [g/mol]: 192.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.07		Crippen Method
logp	-0.197		Crippen Method
mcvol	144.540	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=B6002134&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume