

N-[4-(6-methyl)-1,3,3a,7-tetrazaindenyl]-ethylenediamine 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: DROUECPSPPOUPDI-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/ci9903071>
Crippen Method: https://www.cheméo.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

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