# Adenine, 9-cyclopentyl-, 1-oxide

**Inchi:** InChI=1S/C10H13N5O/c11-9-8-10(13-6-15(9)16)14(5-12-8)7-3-1-2-4-7/h5-7H,1-4,11H2
**InchiKey:** CLSSCSPMNMBTGI-UHFFFAOYSA-N
**Formula:** C10H13N5O
**SMILES:** Nc1c2ncn(C3CCCC3)c2nc[n+]1[O-]
**Mol. weight [g/mol]:** 219.24
**CAS:** 35966-97-3

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -5.34 | | Crippen Method |
| logp | 0.762 | | Crippen Method |
| mcvol | 157.750 | 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=C35966973&Units=SI

## Legend

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