

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:	<chem>Nc1c2ncn(C3CCCC3)c2nc[n+]1[O-]</chem>
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

Latest version available from:

<https://www.chemeo.com/cid/45-992-1/Adenine-9-cyclopentyl-1-oxide.pdf>

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