

9H-purine, 6-amino-9-(2-cyclohexenyl)-

Inchi:	InChI=1S/C11H13N5/c12-10-9-11(14-6-13-10)16(7-15-9)8-4-2-1-3-5-8/h2,4,6-8H,1,3,5H2
InchiKey:	IASJUTNOXFGCJB-UHFFFAOYSA-N
Formula:	C11H13N5
SMILES:	<chem>Nc1ncnc2c1ncn2C1C=CCCC1</chem>
Mol. weight [g/mol]:	215.25
CAS:	6975-25-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.85		Crippen Method
logp	1.690		Crippen Method
mcvol	161.670	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6975253&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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