

Hypoxanthine, 7-cyclopentyl

Inchi:	InChI=1S/C10H12N4O/c15-10-8-9(11-5-12-10)13-6-14(8)7-3-1-2-4-7/h5-7H,1-4H2,(H,11
InchiKey:	JTZOFYHMODHFEF-UHFFFAOYSA-N
Formula:	C10H12N4O
SMILES:	Oc1ncnc2ncn(C3CCCC3)c12
Mol. weight [g/mol]:	204.23
CAS:	40067-43-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.50		Crippen Method
logp	1.647		Crippen Method
mcvol	147.770	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C40067434&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/85-875-7/Hypoxanthine-7-cyclopentyl.pdf>

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