

# Hypoxanthine-9-acetic acid, ethyl ester

<b>Inchi:</b>	InChI=1S/C9H10N4O3/c1-2-16-6(14)3-13-5-12-7-8(13)10-4-11-9(7)15/h4-5H,2-3H2,1H3
<b>InchiKey:</b>	LBXKMPLUVKYWSY-UHFFFAOYSA-N
<b>Formula:</b>	C9H10N4O3
<b>SMILES:</b>	CCOC(=O)Cn1cnc2c(=O)[nH]cnc21
<b>Mol. weight [g/mol]:</b>	222.20
<b>CAS:</b>	55175-33-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.41		Crippen Method
logp	-0.799		Crippen Method
mcvol	151.980	ml/mol	McGowan Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C55175332&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C55175332&amp;Units=SI</a>

## Legend

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

Latest version available from:

<https://www.chemeo.com/cid/45-287-4/Hypoxanthine-9-acetic-acid-ethyl-ester.pdf>

Generated by Cheméo on 2024-04-20 01:57:15.171886044 +0000 UTC m=+15867484.092463356.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.