

# Purine, 1-ethyl-

<b>Inchi:</b>	InChI=1S/C7H8N4/c1-2-11-3-6-7(10-5-11)9-4-8-6/h3-5H,2H2,1H3
<b>InchiKey:</b>	MCKMCFUAOUZPDB-UHFFFAOYSA-N
<b>Formula:</b>	C7H8N4
<b>SMILES:</b>	CCn1cnc2ncnc-2c1
<b>Mol. weight [g/mol]:</b>	148.17
<b>CAS:</b>	7496-45-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.05		Crippen Method
logp	0.798		Crippen Method
mcvol	110.490	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=C7496459&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C7496459&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/57-153-9/Purine-1-ethyl.pdf>

Generated by Cheméo on 2024-05-04 02:19:07.891951407 +0000 UTC m=+17078396.812528723.

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