

# N-Acetylcaprolactam

<b>Other names:</b>	1-Acetylhexahydro-2H-azepin-2-one N-Acetyl-«epsilon»-caprolactam 2H-Azepin-2-one, 1-acetylhexahydro- N-Acetyl-6-caprolactam Acetylcaprolactam Acetylkaprolaktam NSC 522408 N-acetylhexanelactam
<b>Inchi:</b>	InChI=1S/C8H13NO2/c1-7(10)9-6-4-2-3-5-8(9)11/h2-6H2,1H3
<b>InchiKey:</b>	QISSLHPKTCLLDL-UHFFFAOYSA-N
<b>Formula:</b>	C8H13NO2
<b>SMILES:</b>	CC(=O)N1CCCCC1=O
<b>Mol. weight [g/mol]:</b>	155.19
<b>CAS:</b>	1888-91-1

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.19		Crippen Method
logp	0.935		Crippen Method
mvol	125.840	ml/mol	McGowan Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	407.70	K	3.50	NIST Webbook
tbrp	394.50 ± 1.50	K	1.30	NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1888911&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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  
**tbrp:** Boiling point at reduced pressure

Latest version available from:

<https://www.chemeo.com/cid/69-359-8/N-Acetylcaprolactam.pdf>

Generated by Cheméo on 2024-04-24 09:35:39.275309647 +0000 UTC m=+16240588.195886962.

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