N-Acetylcaprolactam

Other names:	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
Inchi:	InChI=1S/C8H13NO2/c1-7(10)9-6-4-2-3-5-8(9)11/h2-6H2,1H3
InchiKey:	QISSLHPKTCLLDL-UHFFFAOYSA-N
Formula:	C8H13NO2
SMILES:	CC(=O)N1CCCCCC1=O
Mol. weight [g/mol]:	155.19
CAS:	1888-91-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.19		Crippen Method
logp	0.935		Crippen Method
mcvol	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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1888911&Units=SI

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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