

2(1H)-Pyridinone, 1-ethyl-

Other names:	2(1H)-Pyridone, 1-ethyl- N-Ethyl-2-pyridone 1-Ethyl-2(1H)pyridone 1-Ethylpyridone 1-Ethyl-2-pyridone 1-Ethyl-2(1H)-pyridinone N-Ethyl-2-pyridinone
Inchi:	InChI=1S/C7H9NO/c1-2-8-6-4-3-5-7(8)9/h3-6H,2H2,1H3
InchiKey:	MTSQHZHIEDRSOM-UHFFFAOYSA-N
Formula:	C7H9NO
SMILES:	CCn1cccc1=O
Mol. weight [g/mol]:	123.15
CAS:	13337-79-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.16		Crippen Method
logp	0.868		Crippen Method
mcvol	101.580	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	408.50 ± 0.50	K	2.70	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13337796&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcpvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure

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