

1-Ethyl-4-piperidone

Other names:	4-Piperidinone, 1-ethyl- 1-ethylpiperidin-4-one
Inchi:	InChI=1S/C7H13NO/c1-2-8-5-3-7(9)4-6-8/h2-6H2,1H3
InchiKey:	BDVKAMAALQXGLM-UHFFFAOYSA-N
Formula:	C7H13NO
SMILES:	CCN1CCC(=O)CC1
Mol. weight [g/mol]:	127.18
CAS:	3612-18-8

Physical Properties

Property code	Value	Unit	Source
hvap	56.70 ± 0.60	kJ/mol	NIST Webbook
log10ws	-0.50		Crippen Method
logp	0.671		Crippen Method
mcvol	110.180	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	320.20	K	0.10	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3612188&Units=SI

Legend

hvap:	Enthalpy of vaporization at standard conditions
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.cheméo.com/cid/17-375-7/1-Ethyl-4-piperidone.pdf>

Generated by Cheméo on 2024-04-24 09:56:24.498746759 +0000 UTC m=+16241833.419324072.

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