

1-Propyl-4-piperidone

Other names:	4-Piperidinone, 1-propyl-
Inchi:	InChI=1S/C8H15NO/c1-2-5-9-6-3-8(10)4-7-9/h2-7H2,1H3
InchiKey:	YGDZKYYCJUNORF-UHFFFAOYSA-N
Formula:	C8H15NO
SMILES:	CCCN1CCC(=O)CC1
Mol. weight [g/mol]:	141.21
CAS:	23133-37-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.92		Crippen Method
logp	1.061		Crippen Method
mcvol	124.270	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	329.20	K	0.10	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23133371&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	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.cheméo.com/cid/29-283-6/1-Propyl-4-piperidone.pdf>

Generated by Cheméo on 2024-04-26 17:12:33.101186066 +0000 UTC m=+16440802.021763388.

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