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/ci990307l
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