1-Allyl-2-(1H)pyridinone

Other names: 1-Allyl-2(1h)-pyridinone
Inchi: InChI=1S/C8H9NO/c1-2-6-9-7-4-3-5-8(9)10/h2-5,7H,1,6H2
InchiKey: QXLAXTADFRGVIS-UHFFFAOYSA-N
Formula: C8H9NO
SMILES: C=CCn1ccccc1=O
Mol. weight [g/mol]: 135.17

Physical Properties

Property code	Value	Unit	Source
ie	8.78	eV	Cheméo Relay (1.0)
log10ws	-0.19		Cheméo Relay (1.0)
logp	1.034		Crippen Method
mcvol	111.370	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	368.00 ± 2.00	K	2.00	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C21997308&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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