5,6-Dehydro-7,9-dihydroxy-7H-pyrrolizineethyl ether

Inchi: InChI=1S/C10H13NO2/c1-2-13-9-4-6-11-5-3-8(7-12)10(9)11/h3-6,9,12H,2,7H2,1H3/t9-/m

InchiKey: IHDSENUTEFTWCP-VIFPVBQESA-N

Formula: C10H13NO2

SMILES: CCOC1C=Cn2ccc(CO)c21

Mol. weight [g/mol]: 179.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.56		Crippen Method
logp	1.542		Crippen Method
mcvol	138.860	ml/mol	McGowan Method
rinpol	1405.00		NIST Webbook
rinpol	1405.00		NIST Webbook

Sources

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=R405228&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

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