

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

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