

# His, 1-methyl, butyl ester

<b>Inchi:</b>	InChI=1S/C11H19N3O2/c1-3-4-5-16-11(15)10(12)6-9-7-14(2)8-13-9/h7-8,10H,3-6,12H2,
<b>InchiKey:</b>	IOXBVOOVLMAXMO-UHFFFAOYSA-N
<b>Formula:</b>	C11H19N3O2
<b>SMILES:</b>	CCCCOC(=O)C(N)Cc1cn(C)cn1
<b>Mol. weight [g/mol]:</b>	225.29

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.83		Crippen Method
logp	0.633		Crippen Method
mcvol	183.770	ml/mol	McGowan Method
rinpol	1888.00		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R31999&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R31999&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>rinpol:</b>	Non-polar retention indices

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