

# L-Histidine, N-(trifluoroacetyl)-, butyl ester

<b>Other names:</b>	His, butyl ester, N-TFA His, butyl ester, TFA
<b>Inchi:</b>	InChI=1S/C12H16F3N3O3/c1-2-3-4-21-10(19)9(5-8-6-16-7-17-8)18-11(20)12(13,14)15/h
<b>InchiKey:</b>	CCHOJMDTLLJCED-VIFPVBQESA-N
<b>Formula:</b>	C12H16F3N3O3
<b>SMILES:</b>	CCCCOC(=O)C(Cc1cnc[nH]1)NC(=O)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	307.27
<b>CAS:</b>	55255-83-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.79		Crippen Method
logp	0.861		Crippen Method
mcvol	204.740	ml/mol	McGowan Method
rinpol	1983.00		NIST Webbook
rinpol	1983.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C55255839&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C55255839&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<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>

## 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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