

L-Histidine, 1-methyl-N-(trifluoroacetyl)-, butyl ester

Other names:	His, 1-methyl-N-(trifluoroacetyl)-, butyl ester His, 3-methyl, butyl ester, TFA
Inchi:	InChI=1S/C13H18F3N3O3/c1-3-4-5-22-11(20)10(18-12(21)13(14,15)16)6-9-7-19(2)8-17
InchiKey:	OGEMYKSAJIDKDR-UHFFFAOYSA-N
Formula:	C13H18F3N3O3
SMILES:	CCCCOC(=O)C(Cc1cn(C)cn1)NC(=O)C(F)(F)F
Mol. weight [g/mol]:	321.30
CAS:	55145-65-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.86		Crippen Method
logp	1.353		Crippen Method
mcvol	218.830	ml/mol	McGowan Method
rinpol	1888.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C55145658&Units=SI

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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