

histidine (monoacyl), trifluoroacetyl-isopropyl ester

Inchi:	InChI=1S/C11H14F3N3O3/c1-6(2)20-9(18)8(3-7-4-15-5-16-7)17-10(19)11(12,13)14/h4-6
InchiKey:	AYAHMTAHALOBDO-UHFFFAOYSA-N
Formula:	C11H14F3N3O3
SMILES:	CC(C)OC(=O)C(Cc1c[nH]cn1)NC(=O)C(F)(F)F
Mol. weight [g/mol]:	293.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.48		Crippen Method
logp	0.469		Crippen Method
mcvol	190.650	ml/mol	McGowan Method
rinpol	1926.00		NIST Webbook
rinpol	1926.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R267893&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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