

Histamine, N-trifluoroacetyl

Other names:	Histamine, N'-trifluoroacetyl-
Inchi:	InChI=1S/C7H8F3N3O/c8-7(9,10)6(14)12-2-1-5-3-11-4-13-5/h3-4H,1-2H2,(H,11,13)(H,12)
InchiKey:	PXVLTDFDQSOFMJ-UHFFFAOYSA-N
Formula:	C7H8F3N3O
SMILES:	O=C(NCCc1c[nH]cn1)C(F)(F)F
Mol. weight [g/mol]:	207.15
CAS:	50580-77-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.72		Crippen Method
logp	0.149		Crippen Method
mcvol	126.850	ml/mol	McGowan Method
rinpola	1636.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C50580773&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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