Histamine, N,N'-di(trifluoroacetyl)-

Inchi: InChI=1S/C9H7F6N3O2/c10-8(11,12)6(19)16-2-1-5-3-18(4-17-5)7(20)9(13,14)15/h3-4H,
InchiKey: CHFXKZMESFCYDT-UHFFFAOYSA-N
Formula: C9H7F6N3O2
SMILES: O=C(NCCc1cn(C(=O)C(F)(F)F)cn1)C(F)(F)F
Mol. weight [g/mol]: 303.16

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.29		Crippen Method
logp	1.307		Crippen Method
mcvol	161.910	ml/mol	McGowan Method
rinpol	1333.00		NIST Webbook
rinpol	1333.00		NIST Webbook

Sources

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=U374887&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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