

Histamine, N'-pentafluoropropionyl-

Inchi: InChI=1S/C8H8F5N3O/c9-7(10,8(11,12)13)6(17)15-2-1-5-3-14-4-16-5/h3-4H,1-2H2,(H,1)
InchiKey: QODSOJCUJPRCLK-UHFFFAOYSA-N
Formula: C8H8F5N3O
SMILES: O=C(NCCc1c[nH]cn1)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 257.16

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.46		Crippen Method
logp	0.784		Crippen Method
mcvol	144.480	ml/mol	McGowan Method
rinpole	1619.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U374888&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/15-087-9/Histamine-N-pentafluoropropionyl.pdf>

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