Histamine, N'-heptafluorobutyryl-

Inchi: InChI=1S/C9H8F7N3O/c10-7(11,8(12,13)9(14,15)16)6(20)18-2-1-5-3-17-4-19-5/h3-4H,1-
InchiKey: IOUCIDQNQUCCBI-UHFFFAOYSA-N
Formula: C9H8F7N3O
SMILES: O=C(NCCc1c[nH]cn1)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 307.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.19		Crippen Method
logp	1.419		Crippen Method
mcvol	162.110	ml/mol	McGowan Method
rinpol	1654.00		NIST Webbook
rinpol	1654.00		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=U374889&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.