Adenine, N4-pentafluoropropionyl-

Inchi: InChI=1S/C8H4F5N5O/c9-7(10,8(11,12)13)6(19)18-5-3-4(15-1-14-3)16-2-17-5/h1-2H,(H2

InchiKey: MDJOJUIOIRMNCK-UHFFFAOYSA-N

Formula: C8H4F5N5O

SMILES: OC(=Nc1ncnc2[nH]cnc12)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 281.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.57		Crippen Method
logp	1.657		Crippen Method
mcvol	144.980	ml/mol	McGowan Method
rinpol	1731.00		NIST Webbook
rinpol	1731.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U374882&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

rinpol: Non-polar retention indices

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