2-Amino-4,6-dihydroxypyrimidine, N,O,O'-tris(pentafluoropropionyl)-

Inchi: InChI=1S/C13H2F15N3O5/c14-8(15,11(20,21)22)4(32)31-7-29-2(35-5(33)9(16,17)12(23

InchiKey: ZAIGGKWWEMSTJZ-UHFFFAOYSA-N

Formula: C13H2F15N3O5

SMILES: O=C(Nc1nc(OC(=O)C(F)(F)C(F)(F)F)cc(OC(=O)C(F)(F)C(F)(F)F)n1)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 565.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.02		Crippen Method
logp	3.819		Crippen Method
mcvol	243.210	ml/mol	McGowan Method
rinpol	1215.00		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=U375760&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