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

Inchi: InChI=1S/C10H2F9N3O5/c11-8(12,13)4(23)22-7-20-2(26-5(24)9(14,15)16)1-3(21-7)27-6

InchiKey: CGILXSBSUZVUGR-UHFFFAOYSA-N

Formula: C10H2F9N3O5

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

Mol. weight [g/mol]: 415.13

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.82		Crippen Method
logp	1.913		Crippen Method
mcvol	190.320	ml/mol	McGowan Method
rinpol	1228.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375761&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices