

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/ci9903071>
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

Latest version available from:

<https://www.chemeo.com/cid/30-619-1/2-Amino-4-6-dihydroxypyrimidine-N-O-O-tris-trifluoroacetyl.pdf>

Generated by Cheméo on 2024-05-03 18:10:09.471927257 +0000 UTC m=+17049058.392504570.

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