4,6-Dihydroxypyrimidine, bis(pentafluoropropionate)

Inchi: InChI=1S/C10H2F10N2O4/c11-7(12,9(15,16)17)5(23)25-3-1-4(22-2-21-3)26-6(24)8(13,1

InchiKey: PMKQNPHJGJZKPG-UHFFFAOYSA-N

Formula: C10H2F10N2O4

SMILES: O=C(Oc1cc(OC(=O)C(F)(F)C(F)(F)F)ncn1)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 404.12

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.42		Crippen Method
logp	2.683		Crippen Method
mcvol	180.540	ml/mol	McGowan Method
rinpol	993.00		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=U375778&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