4,6-Dihydroxypyrimidine, bis(heptafluorobutyrate)

Inchi: InChI=1S/C12H2F14N2O4/c13-7(14,9(17,18)11(21,22)23)5(29)31-3-1-4(28-2-27-3)32-6(

InchiKey: NWMQDVWYPHHXBH-UHFFFAOYSA-N

Formula: C12H2F14N2O4

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

Mol. weight [g/mol]: 504.13

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.89		Crippen Method
logp	3.953		Crippen Method
mcvol	215.800	ml/mol	McGowan Method
rinpol	1072.00		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=U375777&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

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