

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(13,14)20
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/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=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

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<https://www.chemeo.com/cid/51-090-5/4-6-Dihydroxypyrimidine-bis-pentafluoropropionate.pdf>

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