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

Inchi: InChI=1S/C16H2F21N3O5/c17-8(18,11(23,24)14(29,30)31)4(41)40-7-38-2(44-5(42)9(19

InchiKey: YJWNPANTNRJPTP-UHFFFAOYSA-N

Formula: C16H2F21N3O5

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

Mol. weight [g/mol]: 715.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.22		Crippen Method
logp	5.725		Crippen Method
mcvol	296.100	ml/mol	McGowan Method
rinpol	1292.00		NIST Webbook
rinpol	1292.00		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=U375759&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

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