5-Hydroxyindole, N,O-bis(pentafluoropropionyl)-

Inchi: InChI=1S/C14H5F10NO3/c15-11(16,13(19,20)21)9(26)25-4-3-6-5-7(1-2-8(6)25)28-10(27

InchiKey: KPBXVTIYCAQLSU-UHFFFAOYSA-N

Formula: C14H5F10NO3

SMILES: O=C(Oc1ccc2c(ccn2C(=O)C(F)(F)C(F)(F)F)c1)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 425.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.50		Crippen Method
logp	4.582		Crippen Method
mcvol	205.890	ml/mol	McGowan Method
rinpol	1964.00		NIST Webbook
rinpol	1964.00		NIST Webbook

Sources

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=U375685&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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.