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

Inchi: InChI=1S/C16H5F14NO3/c17-11(18,13(21,22)15(25,26)27)9(32)31-4-3-6-5-7(1-2-8(6)31
InchiKey: MOYLBUIZZMOTIC-UHFFFAOYSA-N
Formula: C16H5F14NO3
SMILES: O=C(Oc1ccc2c(ccn2C(=O)C(F)(F)C(F)(F)C(F)(F)F)c1)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 525.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.96		Crippen Method
logp	5.853		Crippen Method
mcvol	241.150	ml/mol	McGowan Method
rinpol	2022.00		NIST Webbook
rinpol	2022.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375684&Units=SI
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

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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