5,5-Diphenylhydantoin, 3-pentafluoropropionyl-

Inchi: InChI=1S/C18H11F5N2O3/c19-17(20,18(21,22)23)14(27)25-13(26)16(24-15(25)28,11-7-

InchiKey: BGMDFPLWEKSBKG-UHFFFAOYSA-N

Formula: C18H11F5N2O3

SMILES: O=C1NC(c2ccccc2)(c2ccccc2)C(=O)N1C(=O)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 398.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.77		Crippen Method
logp	3.206		Crippen Method
mcvol	239.620	ml/mol	McGowan Method
rinpol	2184.00		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=U374834&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