5,5-Diphenylhydantoin. 3-heptafluorobutyryl-

Inchi: InChI=1S/C19H11F7N2O3/c20-17(21,18(22,23)19(24,25)26)14(30)28-13(29)16(27-15(28

InchiKey: STKHQLZUUJTGBP-UHFFFAOYSA-N

Formula: C19H11F7N2O3

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

Mol. weight [g/mol]: 448.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.50		Crippen Method
logp	3.841		Crippen Method
mcvol	257.250	ml/mol	McGowan Method
rinpol	2206.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U374833&Units=SI

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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