

Silane, dimethyl(dimethyl(dimethyl(2-nitrophenoxy)silyloxy)silyloxy)silyloxy-2-nitrophenol

Inchi: InChI=1S/C18H26N2O8Si3/c1-29(2,25-17-13-9-7-11-15(17)19(21)22)27-31(5,6)28-30(3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,25,26,27,28,29,30,31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,47,48,49,50,51,52,53,54,55,56,57,58,59,60,61,62,63,64,65,66,67,68,69,70,71,72,73,74,75,76,77,78,79,80,81,82,83,84,85,86,87,88,89,90,91,92,93,94,95,96,97,98,99,100)/h1-18/t1-3/m0/s1

InchiKey: IABWKUFZEIKRAO-UHFFFAOYSA-N

Formula: C18H26N2O8Si3

SMILES: C[Si](C)(Oc1ccccc1[N+](=O)[O-])O[Si](C)(C)O[Si](C)(C)Oc1ccccc1[N+](=O)[O-]

Mol. weight [g/mol]: 482.66

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.41		Crippen Method
logp	5.099		Crippen Method
rinpol	2672.00		NIST Webbook
rinpol	2672.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U347243&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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