

Butyl

([1,1,3,3,5,5-hexamethyl-5-(pyridin-3-ylmethoxy)trisiloxanyl]oxy)acetate

Other names: Butyl {[1,1,3,3,5,5-hexamethyl-5-(pyridin-3-ylmethoxy)trisiloxanyl]oxy}acetate

Inchi: InChI=1S/C18H35NO6Si3/c1-8-9-13-21-18(20)16-23-27(4,5)25-28(6,7)24-26(2,3)22-15-

InchiKey: DBGOJQAGUHJNOC-UHFFFAOYSA-N

Formula: C18H35NO6Si3

SMILES: CCCCOC(=O)CO[Si](C)(C)O[Si](C)(C)O[Si](C)(C)OCc1ccncc1

Mol. weight [g/mol]: 445.73

Physical Properties

Property code	Value	Unit	Source
log10ws	1.75		Crippen Method
logp	4.097		Crippen Method
rinpol	2233.00		NIST Webbook
rinpol	2233.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U376005&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/114-424-4/Butyl-1-1-3-3-5-5-hexamethyl-5-pyridin-3-ylmethoxy-trisiloxanyl-oxy-acetate>.

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