Phosphoric acid, tris(tert-butyldimethylsilyl) ester

Other names: Tris[tert-butyl(dimethyl)silyl] phosphate

Inchi: InChI=1S/C18H45O4PSi3/c1-16(2,3)24(10,11)20-23(19,21-25(12,13)17(4,5)6)22-26(14,1

InchiKey: XKIUTLXREGOBOW-UHFFFAOYSA-N

Formula: C18H45O4PSi3

SMILES: CC(C)(C)[Si](C)(C)OP(=O)(O[Si](C)(C)C(C)(C)C)O[Si](C)(C)C(C)(C)C

Mol. weight [g/mol]: 440.78

CAS: 85197-28-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.04		Crippen Method
logp	8.160		Crippen Method
rinpol	1938.00		NIST Webbook
rinpol	1924.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C85197280&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

rinpol: Non-polar retention indices

Latest version available from:

https://www.chemeo.com/cid/36-744-6/Phosphoric-acid-tris-tert-butyldimethylsilyl-ester.pdf

Generated by Cheméo on 2024-10-12 03:47:57.526810133 +0000 UTC m=+3285740.163779382.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.