

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(14,15)27-29
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
rinpola	1938.00		NIST Webbook
rinpola	1924.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C85197280&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpola:	Non-polar retention indices

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