Benzaldehyde, 2-hydroxy, 3-nitro-5-tert.-octyl, oxime, TMS

Inchi: InChI=1S/C17H30N2O4Si2/c1-17(2,3)14-10-13(12-18-23-25(7,8)9)16(22-24(4,5)6)15(11

InchiKey: BYXZOFDQJNYVAG-UHFFFAOYSA-N

Formula: C17H30N2O4Si2

SMILES: CC(C)(C)c1cc(C=NO[Si](C)(C)C)c(O[Si](C)(C)C)c([N+](=O)[O-])c1

Mol. weight [g/mol]: 382.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.48		Crippen Method
logp	5.291		Crippen Method
rinpol	2241.00		NIST Webbook

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R58262&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices