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

Inchi: InChI=1S/C21H38ClNO2Si2/c1-20(2,3)15-21(4,5)17-12-16(14-23-25-27(9,10)11)19(18(2

InchiKey: KNOHPLJYSYEMDF-OEAKJJBVSA-N

Formula: C21H38ClNO2Si2

SMILES: CC(C)(C)CC(C)(C)c1cc(Cl)c(O[Si](C)(C)C)c(C=NO[Si](C)(C)C)c1

Mol. weight [g/mol]: 428.16

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.95		Crippen Method
logp	7.453		Crippen Method
rinpol	2105.00		NIST Webbook
rinpol	2107.00		NIST Webbook
rinpol	2105.00		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=R58230&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices