

Benzaldehyde, 2-hydroxy, 3,5-bis-tert.-butyl, oxime, TMS

Inchi: InChI=1S/C21H39NO2Si2/c1-20(2,3)17-13-16(15-22-24-26(10,11)12)19(23-25(7,8)9)18(4,5,6)
InchiKey: GWVUBDVUTDIZEG-PXLXIMEGSA-N
Formula: C21H39NO2Si2
SMILES: CC(C)(C)c1cc(C=NO[Si](C)(C)C)c(O[Si](C)(C)C)c(C(C)(C)C)c1
Mol. weight [g/mol]: 393.71

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.14		Crippen Method
logp	6.681		Crippen Method
rinpol	1937.00		NIST Webbook
rinpol	1937.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R58226&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/39-421-1/Benzaldehyde-2-hydroxy-3-5-bis-tert-butyl-oxime-TMS.pdf>

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