

Benzaldehyde, 3-methoxy-4-[(trimethylsilyl)oxy]-, O-methyloxime

Other names: Vanillin, MO TMS
Inchi: InChI=1S/C12H19NO3Si/c1-14-12-8-10(9-13-15-2)6-7-11(12)16-17(3,4)5/h6-9H,1-5H3
InchiKey: QRZHLXDYKDCOPI-UHFFFAOYSA-N
Formula: C12H19NO3Si
SMILES: CON=Cc1ccc(O[Si](C)(C)C)c(OC)c1
Mol. weight [g/mol]: 253.37
CAS: 55045-03-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.75		Crippen Method
logp	2.889		Crippen Method
rinpol	1619.00		NIST Webbook
rinpol	1619.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C55045039&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/115-733-0/Benzaldehyde-3-methoxy-4-trimethylsilyl-oxy-O-methyloxime.pdf>

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