

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

Other names:	m-Anisaldehyde, 4-(trimethylsiloxy)- Trimethylsilyl vanillin Vanillin, TMS Vanillin, trimethylsilyl ether Vanilline, TMS 3-Methoxy-4-[(trimethylsilyl)oxy]benzaldehyde Vanillin, tms derivative
Inchi:	InChI=1S/C11H16O3Si/c1-13-11-7-9(8-12)5-6-10(11)14-15(2,3)4/h5-8H,1-4H3
InchiKey:	PTXKWJXZIMEWED-UHFFFAOYSA-N
Formula:	C11H16O3Si
SMILES:	<chem>COc1cc(C=O)ccc1O[Si](C)(C)C</chem>
Mol. weight [g/mol]:	224.33
CAS:	6689-43-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.84		Crippen Method
logp	2.721		Crippen Method
rinpol	1530.00		NIST Webbook
rinpol	1529.00		NIST Webbook
rinpol	1544.90		NIST Webbook
rinpol	1494.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6689436&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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.cheméo.com/cid/91-435-8/Benzaldehyde-3-methoxy-4-trimethylsilyl-oxy.pdf>

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