

3-Hydroxy-4-methoxybenzyl alcohol, bis(trimethylsilyl) ether

Other names:

Benzenemethanol, 3-hydroxy-4-methoxy, bis-TMS

Isovanillic alcohol, TMS

3-Hydroxy-4-methoxybenzyl alcohol, 2tms derivative

Inchi:

InChI=1S/C14H26O3Si2/c1-15-13-9-8-12(11-16-18(2,3)4)10-14(13)17-19(5,6)7/h8-10H,1

InchiKey:

IJGZVNYCFGLMLG-UHFFFAOYSA-N

Formula:

C14H26O3Si2

SMILES:

COc1ccc(CO[Si](C)(C)C)cc1O[Si](C)(C)C

Mol. weight [g/mol]:

298.53

Physical Properties

Property code	Value	Unit	Source
log10ws	0.13		Crippen Method
logp	4.260		Crippen Method
rinpol	1626.00		NIST Webbook
rinpol	1627.00		NIST Webbook
rinpol	1624.10		NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U333352&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/36-647-4/3-Hydroxy-4-methoxybenzyl-alcohol-bis-trimethylsilyl-ether.pdf>

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