

Vanillic acid, TBDMS

Other names:	Vanillic acid, diTBDMS
Inchi:	InChI=1S/C20H36O4Si2/c1-19(2,3)25(8,9)23-16-13-12-15(14-17(16)22-7)18(21)24-26(10,11)20
InchiKey:	HKVCRFBFJCHXIE-UHFFFAOYSA-N
Formula:	C20H36O4Si2
SMILES:	COc1cc(C(=O)O[Si](C)(C)C(C)(C)C)ccc1O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	396.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.24		Crippen Method
logp	6.241		Crippen Method
rinpol	2259.00		NIST Webbook
rinpol	2264.00		NIST Webbook
rinpol	2259.00		NIST Webbook
rinpol	2228.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R48681&Units=SI

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/20-199-9/Vanillic-acid-TBDMS.pdf>

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