

Isovanilline, MO TMS

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

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.75		Crippen Method
logp	2.889		Crippen Method
rinpol	1618.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R92595&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.cheméo.com/cid/59-885-5/Isovanilline-MO-TMS.pdf>

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