

3,4,5-Trihydroxybenzoic acid ethyl ester (3TMS)

Inchi:	InChI=1S/C18H34O5Si3/c1-11-20-18(19)14-12-15(21-24(2,3)4)17(23-26(8,9)10)16(13-1
InchiKey:	ILGIXPTYODRSEG-UHFFFAOYSA-N
Formula:	C18H34O5Si3
SMILES:	CCOC(=O)c1cc(O[Si](C)(C)C)c(O[Si](C)(C)C)c(O[Si](C)(C)C)c1
Mol. weight [g/mol]:	414.72

Physical Properties

Property code	Value	Unit	Source
log10ws	0.84		Crippen Method
logp	5.504		Crippen Method
rinpol	1927.40		NIST Webbook
rinpol	1927.40		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=U413962&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

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<https://www.chemeo.com/cid/124-579-2/3-4-5-Trihydroxybenzoic-acid-ethyl-ester-3TMS.pdf>

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