

Benzoic acid, 3,4,5-tris[(trimethylsilyl)oxy]-, propyl ester

Other names:	Propyl gallate, tris(trimethylsilyl) ester Propyl 3,4,5-tris(trimethylsilyloxy)benzoate
Inchi:	InChI=1S/C19H36O5Si3/c1-11-12-21-19(20)15-13-16(22-25(2,3)4)18(24-27(8,9)10)17(1
InchiKey:	WFUMVAGDQRGOTN-UHFFFAOYSA-N
Formula:	C19H36O5Si3
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]:	428.74
CAS:	77160-55-5

Physical Properties

Property code	Value	Unit	Source
log10ws	0.42		Crippen Method
logp	5.895		Crippen Method
rinpol	2050.00		NIST Webbook
rinpol	2050.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C77160555&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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