

Benzoic acid, 2,6-bis[(trimethylsilyl)oxy]-, trimethylsilyl ester

Other names:	2,6-Dihydroxybenzoic acid, bis(trimethylsilyl) ether, trimethylsilyl ester Benzoic acid, 2,6-dihydroxy, tri-TMS Benzoic acid, 2,6-dihydroxy, TMS Trimethylsilyl 2,6-bis[(trimethylsilyl)oxy]benzoate 2,6-Dihydroxybenzoic acid, 3tms derivative
Inchi:	InChI=1S/C16H30O4Si3/c1-21(2,3)18-13-11-10-12-14(19-22(4,5)6)15(13)16(17)20-23(7)
InchiKey:	APVNJYLNHAHELf-UHFFFAOYSA-N
Formula:	C16H30O4Si3
SMILES:	C[Si](C)(C)OC(=O)c1c(O[Si](C)(C)C)cccc1O[Si](C)(C)C
Mol. weight [g/mol]:	370.66
CAS:	3782-85-2

Physical Properties

Property code	Value	Unit	Source
log10ws	1.38		Crippen Method
logp	5.106		Crippen Method
rinpol	1768.00		NIST Webbook
rinpol	1747.60		NIST Webbook
rinpol	1768.00		NIST Webbook
rinpol	1768.00		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=C3782852&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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