

1,3-Benzenedicarboxylic acid, bis(trimethylsilyl) ester

Other names:	Isophthalic acid, 2tms derivative
Inchi:	InChI=1S/C14H22O4Si2/c1-19(2,3)17-13(15)11-8-7-9-12(10-11)14(16)18-20(4,5)6/h7-10
InchiKey:	XBYWPSUAELKTET-UHFFFAOYSA-N
Formula:	C14H22O4Si2
SMILES:	C[Si](C)(C)OC(=O)c1cccc(C(=O)O[Si](C)(C)C)c1
Mol. weight [g/mol]:	310.49
CAS:	106450-31-1

Physical Properties

Property code	Value	Unit	Source
log10ws	0.27		Crippen Method
logp	3.670		Crippen Method
rinpola	1748.00		NIST Webbook
rinpola	1748.00		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=C106450311&Units=SI

Legend

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

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<https://www.chemeo.com/cid/118-313-3/1-3-Benzenedicarboxylic-acid-bis-trimethylsilyl-ester.pdf>

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