

Octan-2-yl trimethylsilyl phthalate

Other names:	1,2-Benzenedicarboxylic acid, octan-2-yl trimethylsilyl ester
Inchi:	InChI=1S/C19H30O4Si/c1-6-7-8-9-12-15(2)22-18(20)16-13-10-11-14-17(16)19(21)23-24
InchiKey:	YNVPHCYRFWQGMX-UHFFFAOYSA-N
Formula:	C19H30O4Si
SMILES:	CCCCCCC(C)OC(=O)c1ccccc1C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	350.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.89		Crippen Method
logp	5.194		Crippen Method
rinpol	2131.00		NIST Webbook
rinpol	2131.00		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=U373695&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.chemeo.com/cid/61-721-3/Octan-2-yl-trimethylsilyl-phthalate.pdf>

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