

Hexyl trimethylsilyl phthalate

Other names:	1,2-Benzenedicarboxylic acid, hexyl trimethylsilyl ester
Inchi:	InChI=1S/C17H26O4Si/c1-5-6-7-10-13-20-16(18)14-11-8-9-12-15(14)17(19)21-22(2,3)4/
InchiKey:	IEVGQLBZCCWXIX-UHFFFAOYSA-N
Formula:	C17H26O4Si
SMILES:	CCCCCOC(=O)c1cccc1C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	322.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.94		Crippen Method
logp	4.415		Crippen Method
rinpol	2027.00		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=U373617&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/31-769-4/Hexyl-trimethylsilyl-phthalate.pdf>

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