

(Z)-Hex-3-enyl trimethylsilyl phthalate

Other names:	1,2-Benzenedicarboxylic acid, (Z)-Hex-3-enyl trimethylsilyl ester
Inchi:	InChI=1S/C17H24O4Si/c1-5-6-7-10-13-20-16(18)14-11-8-9-12-15(14)17(19)21-22(2,3)4/
InchiKey:	XUSGDHULPNXLDO-SREVYHEPSA-N
Formula:	C17H24O4Si
SMILES:	CCC=CCCOC(=O)c1ccccc1C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	320.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.79		Crippen Method
logp	4.191		Crippen Method
rinsol	2022.00		NIST Webbook
rinsol	2022.00		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=U373658&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/34-760-0/Z-Hex-3-enyl-trimethylsilyl-phthalate.pdf>

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