

Pent-4-enyl trimethylsilyl phthalate

Other names:	1,2-Benzenedicarboxylic acid, pent-4-enyl trimethylsilyl ester
Inchi:	InChI=1S/C16H22O4Si/c1-5-6-9-12-19-15(17)13-10-7-8-11-14(13)16(18)20-21(2,3)4/h5,
InchiKey:	KEWYIXVRZBXPON-UHFFFAOYSA-N
Formula:	C16H22O4Si
SMILES:	C=CCCCOC(=O)c1cccc1C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	306.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.37		Crippen Method
logp	3.801		Crippen Method
rinpol	1922.00		NIST Webbook
rinpol	1922.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373655&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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/66-757-9/Pent-4-enyl-trimethylsilyl-phthalate.pdf>

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