

Pentyl trimethylsilyl phthalate

Other names:	1,2-Benzenedicarboxylic acid, pentyl trimethylsilyl ester
Inchi:	InChI=1S/C16H24O4Si/c1-5-6-9-12-19-15(17)13-10-7-8-11-14(13)16(18)20-21(2,3)4/h7-
InchiKey:	YPTDVRWVHFFPMZ-UHFFFAOYSA-N
Formula:	C16H24O4Si
SMILES:	CCCCCOC(=O)c1cccc1C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	308.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.52		Crippen Method
logp	4.025		Crippen Method
rincpol	1930.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373635&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/36-685-2/Pentyl-trimethylsilyl-phthalate.pdf>

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