

Prop-2-ynyl trimethylsilyl phthalate

Other names:	1,2-Benzenedicarboxylic acid, prop-2-ynyl trimethylsilyl ester
Inchi:	InChI=1S/C14H16O4Si/c1-5-10-17-13(15)11-8-6-7-9-12(11)14(16)18-19(2,3)4/h1,6-9H,1
InchiKey:	GSXKMDUROHECTG-UHFFFAOYSA-N
Formula:	C14H16O4Si
SMILES:	C#CCOC(=O)c1ccccc1C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	276.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.48		Crippen Method
logp	2.468		Crippen Method
rinpol	1747.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373669&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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/22-550-6/Prop-2-ynyl-trimethylsilyl-phthalate.pdf>

Generated by Cheméo on 2024-04-29 23:34:35.453694757 +0000 UTC m=+16722924.374272079.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.