

Pentachlorophenol, tert-butyldimethylsilyl ether

Other names:	Pentachlorophenol, TBDMS Pentachlorophenol, tbdms derivative
Inchi:	InChI=1S/C12H15Cl5OSi/c1-12(2,3)19(4,5)18-11-9(16)7(14)6(13)8(15)10(11)17/h1-5H3
InchiKey:	KDPIVORPBWXdGN-UHFFFAOYSA-N
Formula:	C12H15Cl5OSi
SMILES:	CC(C)(C)[Si](C)(C)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	380.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.16		Crippen Method
logp	7.338		Crippen Method
rinpol	2192.70		NIST Webbook
rinpol	2192.70		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333392&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/85-549-9/Pentachlorophenol-tert-butyldimethylsilyl-ether.pdf>

Generated by Cheméo on 2024-04-20 03:04:53.175738608 +0000 UTC m=+15871542.096315919.

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