

O-4-Methyl-2-pentyl, methylphosphonic acid, trimethylsilyl ester

Other names:	Methylphosphonic acid, mono-(4-methyl-2-pentyl) ester, TMS
Inchi:	InChI=1S/C10H25O3PSi/c1-9(2)8-10(3)12-14(4,11)13-15(5,6)7/h9-10H,8H2,1-7H3
InchiKey:	NYSBCRVQKZXXTP-UHFFFAOYSA-N
Formula:	C10H25O3PSi
SMILES:	CC(C)CC(C)OP(C)(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	252.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.38		Crippen Method
logp	4.112		Crippen Method
rinsol	864.00		NIST Webbook
rinsol	864.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U383367&Units=SI

Legend

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

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