

Methylphosphonic acid, mono-(3-methyl-1-butyl) ester, TMS

Other names:	Methylphosphonic acid, 3-methyl-1-butyl, TMS
Inchi:	InChI=1S/C9H23O3PSi/c1-9(2)7-8-11-13(3,10)12-14(4,5)6/h9H,7-8H2,1-6H3
InchiKey:	YQTQITXZRFIYDA-UHFFFAOYSA-N
Formula:	C9H23O3PSi
SMILES:	CC(C)CCOP(C)(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	238.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.85		Crippen Method
logp	3.723		Crippen Method
rinpol	808.00		NIST Webbook
rinpol	808.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R548508&Units=SI

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/73-390-8/Methylphosphonic-acid-mono-3-methyl-1-butyl-ester-TMS.pdf>

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