Isobutyl methylphosphonic acid, TMS derivative

Other names:	Methylphosphonic acid, isobutyl ester, TMS
	Methylphosphonic acid, isobutyl trimethylsilyl ester
	Methylphosphonic acid, mono-isobutyl ester, TMS
Inchi:	InChI=1S/C8H21O3PSi/c1-8(2)7-10-12(3,9)11-13(4,5)6/h8H,7H2,1-6H3
InchiKey:	YKENHQTWUXRYMG-UHFFFAOYSA-N
Formula:	C8H21O3PSi
SMILES:	CC(C)COP(C)(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	224.31
CAS:	199116-09-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.43		Crippen Method
logp	3.333		Crippen Method
rinpol	1221.00		NIST Webbook
rinpol	1221.00		NIST Webbook
rinpol	1214.00		NIST Webbook
rinpol	1221.00		NIST Webbook
rinpol	1214.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C199116091&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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/59-208-6/Isobutyl-methylphosphonic-acid-TMS-derivative.pdf

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