Glyphosate, TBDMS

Inchi:	InChI=1S/C27H64NO5PSi4/c1-24(2,3)35(13,14)28(21-23(29)31-36(15,16)25(4,5)6)22-34
InchiKey:	SETROWTYASRSNP-UHFFFAOYSA-N
Formula:	C27H64NO5PSi4
SMILES:	CC(C)(C)[Si](C)(C)OC(=O)CN(CP(=O)(O[Si](C)(C)C(C)(C)C)O[Si](C)(C)C(C)(C)C)[Si](C)
Mol. weight [g/mol]:	626.12

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.70		Crippen Method
logp	10.036		Crippen Method
rinpol	2436.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R76050&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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/53-377-5/Glyphosate-TBDMS.pdf

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