Indole-3-pyruvic acid, TMS

Inchi:	InChI=1S/C23H41NO4Si4/c1-29(2,3)24-17-18(20-16-19(13-14-21(20)24)26-30(4,5)6)15-
InchiKey:	LLCPITUOMNTHRE-JCMHNJIXSA-N
Formula:	C23H41NO4Si4
SMILES:	C[Si](C)(C)OC(=O)C(=Cc1cn([Si](C)(C)C)c2ccc(O[Si](C)(C)C)cc12)O[Si](C)(C)C
Mol. weight [g/mol]:	507.92

Physical Properties

Property code	Value	Unit	Source
log10ws	1.08		Crippen Method
logp	7.109		Crippen Method
rinpol	2433.00		NIST Webbook
rinpol	2433.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R485848&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

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https://www.chemeo.com/cid/48-939-7/Indole-3-pyruvic-acid-TMS.pdf
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