Echimidine, triTMS

Inchi:	InChI=1S/C29H55NO7Si3/c1-15-21(2)26(31)34-24-17-19-30-18-16-23(25(24)30)20-33-2
InchiKey:	WVGXXUANQZAHGA-DDNZYNPUSA-N
Formula:	C29H55NO7Si3
SMILES:	CC=C(C)C(=O)OC1CCN2CC=C(COC(=O)C(O[Si](C)(C)C)(C(C)O[Si](C)(C)C)C(C)(C)O[
Mol. weight [g/mol]:	614.01

Physical Properties

Property code	Value	Unit	Source
log10ws	0.27		Crippen Method
logp	5.882		Crippen Method
rinpol	2823.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R252425&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/49-703-7/Echimidine-triTMS.pdf

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