Pantoyl lactone, trimethylsilyl

Other names:	Pantolactone, mono-TMS 2(3H)-Furanone, dihydro-4,4-dimethyl-3-[(trimethylsilyl)oxy]-, (3R)- 4,4-Dimethyl-3-[(trimethylsilyl)oxy]dihydro-2(3H)-furanone, (3R)- Pantolactone, (3r)-, tms derivative
Inchi:	InChI=1S/C9H18O3Si/c1-9(2)6-11-8(10)7(9)12-13(3,4)5/h7H,6H2,1-5H3
InchiKey:	FHABWLGAZORNTC-UHFFFAOYSA-N
Formula:	C9H18O3Si
SMILES:	CC1(C)COC(=O)C1O[Si](C)(C)C
Mol. weight [g/mol]:	202.32
CAS:	42411-50-7

Physical Properties

Property code	Value	Unit	Source
log10ws	0.64		Crippen Method
logp	1.789		Crippen Method
rinpol	1168.00		NIST Webbook
rinpol	1195.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C42411507&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

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