Hexestrol, di-TMS

Other names:	Shikimic acid, TMS
	Hexestrol, 2tms derivative
Inchi:	InChI=1S/C24H38O2Si2/c1-9-23(19-11-15-21(16-12-19)25-27(3,4)5)24(10-2)20-13-17-2
InchiKey:	MADNHYZLYYPMRE-UHFFFAOYSA-N
Formula:	C24H38O2Si2
SMILES:	CCC(c1ccc(O[Si](C)(C)C)cc1)C(CC)c1ccc(O[Si](C)(C)C)cc1
Mol. weight [g/mol]:	414.73
CAS:	70244-15-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.51		Crippen Method
logp	7.801		Crippen Method
rinpol	1842.00		NIST Webbook
rinpol	1849.00		NIST Webbook
rinpol	1849.00		NIST Webbook
rinpol	1849.00		NIST Webbook
rinpol	1860.00		NIST Webbook
rinpol	1864.00		NIST Webbook
rinpol	1865.00		NIST Webbook
rinpol	1865.00		NIST Webbook
rinpol	1844.00		NIST Webbook
rinpol	1825.00		NIST Webbook
rinpol	1839.00		NIST Webbook
rinpol	1849.00		NIST Webbook
rinpol	1826.00		NIST Webbook
rinpol	1836.00		NIST Webbook
rinpol	1846.00		NIST Webbook
rinpol	1842.00		NIST Webbook
rinpol	1864.00		NIST Webbook
rinpol	1839.00		NIST Webbook
rinpol	1825.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C70244154&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