

Methoxyoestrone (enol)-TMS

Other names:	4-Methoxyoestrone, TMS
Inchi:	InChI=1S/C25H40O3Si2/c1-25-16-15-18-17-11-13-22(27-29(3,4)5)24(26-2)20(17)10-9-1
InchiKey:	OUBUBDDLNRBPBN-AAANETGISA-N
Formula:	C25H40O3Si2
SMILES:	COc1c(O[Si](C)(C)C)ccc2c1CCC1C2CCC2(C)C(O[Si](C)(C)C)=CCC12
Mol. weight [g/mol]:	444.75

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.22		Crippen Method
logp	7.110		Crippen Method
rinpola	2687.00		NIST Webbook
rinpola	2634.00		NIST Webbook
rinpola	2687.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R166408&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
rinpola:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/21-191-6/Methoxyoestrone-enol-TMS.pdf>

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