

# Estra-1,3,5(10)-trien-17-one, 2-methoxy-3-[(trimethylsilyl)oxy]-

**Other names:** Mono(trimethylsilyl) derivative of 2-Methoxy-estrone

2-Methoxyestrone, 3-trimethylsilyl ether

**Inchi:** InChI=1S/C22H32O3Si/c1-22-11-10-15-16(18(22)8-9-21(22)23)7-6-14-12-20(25-26(3,4)5

**InchiKey:** PFSHHZVOBSTPMI-UHFFFAOYSA-N

**Formula:** C22H32O3Si

**SMILES:** COc1cc2c(cc1O[Si](C)(C)C)CCC1C2CCC2(C)C(=O)CCC12

**Mol. weight [g/mol]:** 372.57

**CAS:** 29825-40-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.76		Crippen Method
logp	5.334		Crippen Method
rinpola	2815.40		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C29825409&Units=SI>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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

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