

2-Methoxy-3,16,17-tris[(trimethylsilyl)oxy]estra-1,3,5(10)-triene-16 α ,17 β)-diol

Other names: 2-Methoxy-3,16,17-tris[(trimethylsilyl)oxy]estra-1,3,5(10)-triene-16 α ,17 β)-diol, 2-Methoxyoestriol, (4-TMS)-, 2-Methoxyoestriol, TMS, 2-Methoxyestriol, 3tms derivative

Inchi: InChI=1S/C28H50O4Si3/c1-28-15-14-20-21(23(28)18-26(31-34(6,7)8)27(28)32-35(9,10)24)/p1

InchiKey: GUXLPKBCBNPNSW-KTCYKHMTSA-N

Formula: C28H50O4Si3

SMILES: COc1cc2c(cc1O[Si](C)(C)C)CCC1C2CCC2(C)C1CC(O[Si](C)(C)C)C2O[Si](C)(C)C

Mol. weight [g/mol]: 534.95

CAS: 51497-48-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.49		Crippen Method
logp	7.815		Crippen Method

Sources

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

Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C51497484&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

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