17.alpha.-Ethynylestradiol, bis(trimethylsilyl) ether

Other names: 17«alpha»-Ethynyl-3,17-bis[(trimethylsilyl)oxy]estra-1,3,5(10)-triene, (17«beta»)-
17«alpha»-Ethynylestradiol, bis(trimethylsilyl) ether
Ethinylestradiol, bis-TMS
Ethinylestradiol, TMS
Ethinyl estradiol, 2tms derivative

Inchi: InChI=1S/C26H40O2Si2/c1-9-26(28-30(6,7)8)17-15-24-23-12-10-19-18-20(27-29(3,4)5)1

InchiKey: JERDCJZDIHZFGT-PUHDZGQXSA-N

Formula: C26H40O2Si2

SMILES: C#C[C@@]1(O[Si](C)(C)C)CC[C@H]2[C@@H]3CCc4cc(O[Si](C)(C)C)ccc4[C@H]3CC[

Mol. weight [g/mol]: 440.78

Physical Properties

Property code	Value	Unit	Source
ie	8.13	eV	Cheméo Relay (1.0)
log10ws	-6.47		Cheméo Relay (1.0)
logp	6.980		Crippen Method
tf	407.85	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?Str2File=C28426359

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

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

Cheméo Relay (1.0):

Legend

ie: Ionization energy

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

tf: Normal melting (fusion) point