

17«alpha»-Ethinylestradiol, 3-(tert-butyl dimethylsilyl) ether

Other names:	Ethinyl estradiol, tbdms derivative
Inchi:	InChI=1S/C26H38O2Si/c1-8-26(27)16-14-23-22-11-9-18-17-19(28-29(6,7)24(2,3)4)10-12
InchiKey:	CSZIVCGZGDDUNR-UHFFFAOYSA-N
Formula:	C26H38O2Si
SMILES:	C#CC1(O)CCC2C3CCc4cc(O[Si](C)(C)C(C)(C)C)ccc4C3CCC21C
Mol. weight [g/mol]:	410.66

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.62		Crippen Method
logp	6.291		Crippen Method
rinpol	3024.70		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352390&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

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<https://www.chemeo.com/cid/43-646-7/17-alpha-Ethinylestradiol-3-tert-butyl dimethylsilyl-ether.pdf>

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