

Ergostatetraenol, trimethylsilyl

Other names:	Ergosta-5,7,22,24(28)-tetraen-3«beta»-ol, TMS
Inchi:	InChI=1S/C31H50OSi/c1-21(2)22(3)10-11-23(4)27-14-15-28-26-13-12-24-20-25(32-33(7
InchiKey:	GNIWMAVRDVBAL-XAGLJQQCSA-N
Formula:	C31H50OSi
SMILES:	C=C(C=CC(C)C1CCC2C3=CC=C4CC(O[Si](C)(C)C)CCC4(C)C3CCC21C)C(C)C
Mol. weight [g/mol]:	466.81
CAS:	62108-12-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.35		Crippen Method
logp	9.110		Crippen Method
rinpol	3219.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C62108127&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/81-560-0/Ergostatetraenol-trimethylsilyl.pdf>

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