

Dehydroepiandrosterone MO TMS

Other names:	5-Androsten-3«beta»-ol-17-one (Dehydroepiandrosterone), MO-TMS
Inchi:	InChI=1S/C23H39NO2Si/c1-22-13-11-17(26-27(4,5)6)15-16(22)7-8-18-19-9-10-21(24-25)23
InchiKey:	UIADQMRCKCZPLA-JPJGLVNUSA-N
Formula:	C23H39NO2Si
SMILES:	CON=C1CCC2C3CCC4=CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	389.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.17		Crippen Method
logp	6.172		Crippen Method
rinpol	2563.00		NIST Webbook
rinpol	2557.00		NIST Webbook
rinpol	2579.00		NIST Webbook
rinpol	2625.00		NIST Webbook
rinpol	2590.00		NIST Webbook
rinpol	2582.00		NIST Webbook
rinpol	2542.00		NIST Webbook
rinpol	2596.00		NIST Webbook
rinpol	2599.00		NIST Webbook
rinpol	2563.00		NIST Webbook
rinpol	2622.00		NIST Webbook
rinpol	2563.00		NIST Webbook
rinpol	2590.00		NIST Webbook
rinpol	2563.00		NIST Webbook
rinpol	2622.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R92684&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

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