

trans-Dehydroandrosterone, trimethylsilyl ether, O-methyloxime

Other names:	DHEA, 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)
InchiKey:	ZUCRMUCINLDBSB-UHFFFAOYSA-N
Formula:	C23H39NO2Si
SMILES:	CON=C1CCC2C3CC=C4CC(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	2631.00		NIST Webbook
rinpol	2634.00		NIST Webbook
rinpol	2631.00		NIST Webbook
rinpol	2634.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U394495&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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/119-402-3/trans-Dehydroandrosterone-trimethylsilyl-ether-O-methyloxime.pdf>

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