

Lup-20(29)-en-28-al, 3-(trimethylsilyl)oxy, (3«beta»)-

Inchi:	InChI=1S/C33H56O2Si/c1-22(2)23-13-18-33(21-34)20-19-31(6)24(28(23)33)11-12-26-30
InchiKey:	BSQAHRXJLOWUFI-UHFFFAOYSA-N
Formula:	C33H56O2Si
SMILES:	C=C(C)C1CCC2(C=O)CCC3(C)C(CCC4C5(C)CCC(O[Si](C)(C)C)C(C)(C)C5CCC43C)C
Mol. weight [g/mol]:	512.88

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.08		Crippen Method
logp	9.063		Crippen Method
rinpol	3610.00		NIST Webbook
rinpol	3610.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U414392&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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/97-220-0/Lup-20-29-en-28-al-3-trimethylsilyl-oxy-3-beta.pdf>

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