

«beta»-Amyrin trimethylsilyl ether

Other names:	Silane, trimethyl[[(3«beta»)-olean-12-en-3-yl]oxy]- Silane, trimethyl(olean-12-en-3«beta»-yloxy)- «beta»-Amyrin, TMS 3-[(Trimethylsilyl)oxy]olean-12-ene «BETA»-amyrin, tms derivative
Inchi:	InChI=1S/C33H58OSi/c1-28(2)18-19-30(5)20-21-32(7)23(24(30)22-28)12-13-26-31(6)16
InchiKey:	DTNMLCLEKOLKGE-UHFFFAOYSA-N
Formula:	C33H58OSi
SMILES:	CC1(C)CCC2(C)CCC3(C)C(=CCC4C5(C)CCC(O[Si](C)(C)C)C(C)(C)C5CCC43C)C2C1
Mol. weight [g/mol]:	498.90
CAS:	1721-67-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.04		Crippen Method
logp	10.028		Crippen Method
rinpol	3348.00		NIST Webbook
rinpol	3385.00		NIST Webbook
rinpol	3348.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1721671&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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