Cohulupone, TMS

Inchi:	InChI=1S/C22H34O4Si/c1-14(2)10-12-22(13-11-15(3)4)20(24)17(18(23)16(5)6)19(21(22
InchiKey:	BPJDNHJLOXBFDH-UHFFFAOYSA-N
Formula:	C22H34O4Si
SMILES:	CC(C)=CCC1(CC=C(C)C)C(=O)C(O[Si](C)(C)C)=C(C(=O)C(C)C)C1=O
Mol. weight [g/mol]:	390.59

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.48		Crippen Method
logp	5.168		Crippen Method
rinpol	2039.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R305514&Units=SI

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/54-991-2/Cohulupone-TMS.pdf

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