

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R305514&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

Latest version available from:

<https://www.chemeo.com/cid/54-991-2/Cohulupone-TMS.pdf>

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