

cis-Isoadhumulone, TMS

Inchi: InChI=1S/C27H46O5Si2/c1-13-20(6)24(29)23-25(30)21(16-14-18(2)3)27(32-34(10,11)12
InchiKey: QHGGPAUBGUQBCS-COWGUHPFSA-N
Formula: C27H46O5Si2
SMILES: CCC(C)C(=O)C1=C(O[Si](C)(C)C)C(O[Si](C)(C)C)(C(=O)CC=C(C)C)C(CC=C(C)C)C1=C
Mol. weight [g/mol]: 506.82

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.82		Crippen Method
logp	6.778		Crippen Method
rinpol	2652.00		NIST Webbook
rinpol	2603.00		NIST Webbook
rinpol	2652.00		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=R96959&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/45-146-0/cis-Isoadhumulone-TMS.pdf>

Generated by Cheméo on 2025-12-05 11:16:35.738693612 +0000 UTC m=+4681593.268734266.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.