

cis-Isocohumulone, TMS

Inchi: InChI=1S/C28H52O4Si3/c1-20(2)16-17-23-26(30-33(7,8)9)24(25(29)22(5)6)27(31-34(10
InchiKey: NSTHGABYXVJJHV-UHFFFAOYSA-N
Formula: C28H52O4Si3
SMILES: CC(C)=CCC1=C(O[Si](C)(C)C)C(C(=O)C(C)C)=C(O[Si](C)(C)C)C1(CC=C(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 536.97

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.41		Crippen Method
logp	8.739		Crippen Method
rinpol	2597.00		NIST Webbook
rinpol	2572.00		NIST Webbook
rinpol	2554.00		NIST Webbook
rinpol	2528.00		NIST Webbook
rinpol	2554.00		NIST Webbook
rinpol	2597.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R96963&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/121-920-5/cis-Isocohumulone-TMS.pdf>

Generated by Cheméo on 2024-04-23 19:30:11.57746475 +0000 UTC m=+16189860.498042062.

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