

cis-Cohumulinic acid, TMS

Inchi: InChI=1S/C23H44O4Si3/c1-16(2)14-15-18-21(25-28(5,6)7)19(20(24)17(3)4)23(27-30(11
InchiKey: FBRQFRXILTUOPG-UHFFFAOYSA-N
Formula: C23H44O4Si3
SMILES: CC(C)=CCC1=C(O[Si](C)(C)C)C(C(=O)C(C)C)=C(O[Si](C)(C)C)C1O[Si](C)(C)C
Mol. weight [g/mol]: 468.85

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.46		Crippen Method
logp	7.013		Crippen Method
rinsol	2183.00		NIST Webbook
rinsol	2152.00		NIST Webbook
rinsol	2184.00		NIST Webbook
rinsol	2118.00		NIST Webbook
rinsol	2125.00		NIST Webbook
rinsol	2142.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemed.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R96931&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinsol: Non-polar retention indices

Latest version available from:

<https://www.chemed.com/cid/21-455-3/cis-Cohumulinic-acid-TMS.pdf>

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