

trans-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-PNSJCDHTSA-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	2607.00		NIST Webbook
rinpol	2569.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R97125&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/26-105-6/trans-Isoadhumulone-TMS.pdf>

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