

7«beta»-Hydroxy kaurenoic acid, TMS

Inchi: InChI=1S/C26H46O3Si2/c1-18-16-26-17-19(18)11-12-20(26)24(2)13-10-14-25(3,23(27)28)
InchiKey: JNEQSDCDOJSIRI-CGRGLJNGSA-N
Formula: C₂₆H₄₆O₃Si₂
SMILES: C=C1CC23CC1CCC2C1(C)CCCC(C)(C(=O)O[Si](C)(C)C)C1CC3O[Si](C)(C)C
Mol. weight [g/mol]: 462.81

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.85		Crippen Method
logp	7.164		Crippen Method
rinpol	2552.00		NIST Webbook
rinpol	2557.00		NIST Webbook
rinpol	2552.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R559083&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/29-730-9/7-beta-Hydroxy-kaurenoic-acid-TMS.pdf>

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