

Germitorosone, TMS

Inchi: InChI=1S/C29H50O6Si4/c1-19-22(31-3)17-20-16-21-18-29(2,35-39(13,14)15)28(34-38(1
InchiKey: LIJKJWJXYBVZCT-UHFFFAOYSA-N
Formula: C29H50O6Si4
SMILES: COc1cc2cc3c(c(O[Si](C)(C)C)c2c(O[Si](C)(C)C)c1C)C(=O)C(O[Si](C)(C)C)C(C)(O[Si](C)
Mol. weight [g/mol]: 607.05

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.68		Crippen Method
logp	8.153		Crippen Method
rinpol	2800.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R158244&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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/18-316-1/Germitorosone-TMS.pdf>

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