

GA4-diacid, methyl ester TMS ether

Inchi: InChI=1S/C27H46O6Si2/c1-17-15-26-16-18(17)11-12-19(26)27(33-35(8,9)10)14-13-20(3)
InchiKey: CPTRWDMUFIOHKD-QGPPGHEHSA-N
Formula: C27H46O6Si2
SMILES: C=C1CC23CC1CCC2C1(O[Si](C)(C)C)CCC(O[Si](C)(C)C)C(C)(C(=O)OC)C1C3C(=O)O
Mol. weight [g/mol]: 522.82

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.33		Crippen Method
logp	5.551		Crippen Method
rinpol	2425.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R181378&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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.cheméo.com/cid/25-568-4/GA4-diacid-methyl-ester-TMS-ether.pdf>

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