

Antheridic acid, MeTMS

Inchi: InChI=1S/C26H40O6Si2/c1-15-16-10-12-25(21(15)32-34(7,8)9)17(14-16)19(22(27)29-3)
InchiKey: JTMLNMMXXFILOY-GKNFULMRSA-N
Formula: C26H40O6Si2
SMILES: C=C1C2C=C3C(C(=O)OC)C4C5(C)C(=O)OC4(CCC5O[Si](C)(C)C)C3(CC2)C1O[Si](C)(C)C
Mol. weight [g/mol]: 504.76

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.02		Crippen Method
logp	4.834		Crippen Method
rinpol	2730.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R181472&Units=SI>

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/32-398-5/Antheridic-acid-MeTMS.pdf>

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