

[13C] GA58 methyl ester TMS ether

Inchi: InChI=1S/C26H42O6Si2/c1-15-13-25-14-16(15)17(31-33(4,5)6)12-18(25)26-11-10-19(32)
InchiKey: YJIAMACEKPLATL-XJFMSQKNSA-N
Formula: C26H42O6Si2
SMILES: C=C1CC23CC1C(O[Si](C)(C)C)CC2C12CCC(O[Si](C)(C)C)C(C)(C(=O)O1)C2C3C(=O)C
Mol. weight [g/mol]: 506.78

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.92		Crippen Method
logp	4.914		Crippen Method
rinpol	2738.00		NIST Webbook
rinpol	2727.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R176891&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/69-676-6/13C-GA58-methyl-ester-TMS-ether.pdf>

Generated by Cheméo on 2024-04-29 05:31:35.583583514 +0000 UTC m=+16657944.504160830.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.