

[14C4]GA25 methyl ester

Inchi: InChI=1S/C25H38O6Si/c1-15-13-24-14-16(15)9-10-17(24)25(22(28)31-32(5,6)7)12-8-11
InchiKey: SIULXVUBVYCKBA-QIVWLPTESA-N
Formula: C25H38O6Si
SMILES: C=C1CC23CC1CCC2C1(C(=O)O[Si](C)(C)C)CCCC(C)(C(=O)OC)C1C3C(=O)OC
Mol. weight [g/mol]: 462.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.67		Crippen Method
logp	4.496		Crippen Method
rinpol	2438.00		NIST Webbook
rinpol	2438.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R392964&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/26-983-2/14C4-GA25-methyl-ester.pdf>

Generated by Cheméo on 2024-04-26 20:19:58.110334173 +0000 UTC m=+16452047.030911488.

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