

[14C] GA62 methyl ester TMS ether

Inchi: InChI=1S/C23H32O5Si/c1-13-11-22-12-14(13)7-8-15(22)23-16(28-29(4,5)6)9-10-21(2,20)
InchiKey: OWKLDICCFUHXEP-WKIVUHLDSA-N
Formula: C23H32O5Si
SMILES: C=C1CC23CC1CCC2C12OC(=O)C(C)(C=CC1O[Si](C)(C)C)C2C3C(=O)OC
Mol. weight [g/mol]: 416.58

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.27		Crippen Method
logp	3.860		Crippen Method
rinsol	2424.00		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R190926&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
rinsol: Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/43-373-0/14C-GA62-methyl-ester-TMS-ether.pdf>

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