

[13C]GA51, MeTMS

Inchi: InChI=1S/C23H34O5Si/c1-13-9-22-10-14(13)7-8-16(22)23-12-15(28-29(4,5)6)11-21(2,20)
InchiKey: SZCXNKBZPNFVSY-XXMNCVSDSA-N
Formula: C23H34O5Si
SMILES: C=C1CC23CC1CCC2C12CC(O[Si](C)(C)C)CC(C)(C(=O)O1)C2C3C(=O)OC
Mol. weight [g/mol]: 418.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.41		Crippen Method
logp	4.084		Crippen Method
rinpol	2518.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R270176&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/45-141-5/13C-GA51-MeTMS.pdf>

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