

GA4 MeTMS

Other names: GA4 methyl ester TMS ether
GA4, methyl ester TMS
Gibberelline GA4, methyl ester TMS ether
Gibberellin GA4, methyl ester trimethylsilyl ether

Inchi: InChI=1S/C23H34O5Si/c1-13-11-22-12-14(13)7-8-15(22)23-10-9-16(28-29(4,5)6)21(2,20

InchiKey: ATWIBZVZMYFKOI-JKQFYZDSSA-N

Formula: C₂₃H₃₄O₅Si

SMILES: C=C1CC23CC1CCC2C12CCC(O[Si](C)(C)C)C(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	2498.00		NIST Webbook
rinpol	2514.00		NIST Webbook
rinpol	2528.00		NIST Webbook
rinpol	2528.00		NIST Webbook
rinpol	2522.00		NIST Webbook
rinpol	2506.00		NIST Webbook
rinpol	2506.00		NIST Webbook
rinpol	2500.00		NIST Webbook
rinpol	2503.00		NIST Webbook
rinpol	2515.00		NIST Webbook
rinpol	2507.00		NIST Webbook
rinpol	2509.00		NIST Webbook
rinpol	2522.00		NIST Webbook
rinpol	2522.00		NIST Webbook
rinpol	2510.00		NIST Webbook
rinpol	2493.00		NIST Webbook
rinpol	2501.00		NIST Webbook
rinpol	2502.00		NIST Webbook
rinpol	2519.00		NIST Webbook
rinpol	2496.00		NIST Webbook
rinpol	2497.00		NIST Webbook
rinpol	2510.00		NIST Webbook
rinpol	2497.00		NIST Webbook

rinpol	2501.00	NIST Webbook
rinpol	2502.00	NIST Webbook
rinpol	2500.00	NIST Webbook
rinpol	2528.00	NIST Webbook
rinpol	2484.00	NIST Webbook
rinpol	2518.00	NIST Webbook
rinpol	2520.00	NIST Webbook
rinpol	2521.00	NIST Webbook
rinpol	2521.00	NIST Webbook
rinpol	2521.00	NIST Webbook
rinpol	2533.00	NIST Webbook
rinpol	2499.00	NIST Webbook
rinpol	2504.00	NIST Webbook
rinpol	2509.00	NIST Webbook
rinpol	2546.00	NIST Webbook
rinpol	2490.00	NIST Webbook
rinpol	2489.00	NIST Webbook
rinpol	2508.00	NIST Webbook
rinpol	2493.00	NIST Webbook
rinpol	2493.00	NIST Webbook
rinpol	2493.00	NIST Webbook
rinpol	2493.00	NIST Webbook
rinpol	2528.00	NIST Webbook
rinpol	2521.00	NIST Webbook
rinpol	2509.00	NIST Webbook
rinpol	2493.00	NIST Webbook
rinpol	2522.00	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=R79636&Units=SI>

Legend

log10ws:

Log10 of Water solubility in mol/l

logp:

Octanol/Water partition coefficient

rinpol:

Non-polar retention indices

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