GA3, MeTMSi

Other names: GA3 methyl ester TMS ether
GA3, MeTMS
GA3, methyl ester TMS
Gibberellic acid, MeTMS

Inchi: InChI=1S/C26H40O6Si2/c1-16-14-24-15-25(16,32-34(7,8)9)12-10-17(24)26-13-11-18(31

InchiKey: QJSHIGDRCGMRDL-RWHUMPPASA-N

Formula: C26H40O6Si2

SMILES: C=C1CC23CC1(O[Si](C)(C)C)CCC2C12C=CC(O[Si](C)(C)C)C(C)(C(=O)O1)C2C3C(=O)

Mol. weight [g/mol]: 504.76

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.02		Crippen Method
logp	4.834		Crippen Method
rinpol	2692.00		NIST Webbook
rinpol	2752.00		NIST Webbook
rinpol	2746.00		NIST Webbook
rinpol	2746.00		NIST Webbook
rinpol	2750.00		NIST Webbook
rinpol	2692.00		NIST Webbook
rinpol	2729.00		NIST Webbook
rinpol	2730.00		NIST Webbook
rinpol	2729.00		NIST Webbook
rinpol	2730.00		NIST Webbook
rinpol	2692.00		NIST Webbook
rinpol	2712.00		NIST Webbook
rinpol	2713.00		NIST Webbook
rinpol	2692.00		NIST Webbook
rinpol	2699.00		NIST Webbook
rinpol	2696.00		NIST Webbook
rinpol	2696.00		NIST Webbook
rinpol	2686.00		NIST Webbook
rinpol	2697.00		NIST Webbook
rinpol	2692.00		NIST Webbook
rinpol	2699.00		NIST Webbook
rinpol	2712.00		NIST Webbook
rinpol	2713.00		NIST Webbook

rinpol	2700.00	NIST Webbook
rinpol	2692.00	NIST Webbook
rinpol	2693.00	NIST Webbook
rinpol	2692.00	NIST Webbook
rinpol	2686.00	NIST Webbook
rinpol	2706.00	NIST Webbook
rinpol	2707.00	NIST Webbook
rinpol	2672.00	NIST Webbook
rinpol	2673.00	NIST Webbook
rinpol	2695.00	NIST Webbook
rinpol	2695.00	NIST Webbook
rinpol	2714.00	NIST Webbook
rinpol	2714.00	NIST Webbook
rinpol	2693.00	NIST Webbook
rinpol	2694.00	NIST Webbook
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rinpol	2702.00	NIST Webbook
rinpol	2708.00	NIST Webbook
rinpol	2713.00	NIST Webbook
rinpol	2704.00	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R79529&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/30-485-0/GA3-MeTMSi.pdf

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