

GA5, MeTMS

Other names: GA5 methyl ester TMS ether
Inchi: InChI=1S/C23H32O5Si/c1-14-12-21-13-22(14,28-29(4,5)6)11-8-15(21)23-10-7-9-20(2,19)
InchiKey: JKQCNZHRNGPPQX-VMEUSVKSSA-N
Formula: C₂₃H₃₂O₅Si
SMILES: C=C1CC23CC1(O[Si](C)(C)C)CCC2C12CC=CC(C)(C(=O)O1)C2C3C(=O)OC
Mol. weight [g/mol]: 416.58

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.51		Crippen Method
logp	4.004		Crippen Method
rinpol	2534.00		NIST Webbook
rinpol	2513.00		NIST Webbook
rinpol	2485.00		NIST Webbook
rinpol	2512.00		NIST Webbook
rinpol	2513.00		NIST Webbook
rinpol	2495.00		NIST Webbook
rinpol	2510.00		NIST Webbook
rinpol	2510.00		NIST Webbook
rinpol	2476.00		NIST Webbook
rinpol	2512.00		NIST Webbook
rinpol	2534.00		NIST Webbook
rinpol	2534.00		NIST Webbook
rinpol	2534.00		NIST Webbook
rinpol	2534.00		NIST Webbook
rinpol	2534.00		NIST Webbook
rinpol	2466.00		NIST Webbook
rinpol	2534.00		NIST Webbook
rinpol	2482.00		NIST Webbook
rinpol	2479.00		NIST Webbook
rinpol	2482.00		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=R79743&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/47-120-6/GA5-MeTMS.pdf>

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