

GA62, MeTMS

Other names: 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-CIDOZKHUSA-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
rinpol	2424.00		NIST Webbook
rinpol	2419.00		NIST Webbook
rinpol	2439.00		NIST Webbook
rinpol	2418.00		NIST Webbook
rinpol	2420.00		NIST Webbook
rinpol	2422.00		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=R79775&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/68-067-3/GA62-MeTMS.pdf>

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