

GA20 ethyl ester, TMS

Inchi: InChI=1S/C24H36O5Si/c1-7-27-19(25)17-18-21(3)10-8-11-24(18,28-20(21)26)16-9-12-2
InchiKey: UJGBPMZRWPCHOH-LEWAGNQXSA-N
Formula: C24H36O5Si
SMILES: C=C1CC23CC1(O[Si](C)(C)C)CCC2C12CCCC(C)(C(=O)O1)C2C3C(=O)OCC
Mol. weight [g/mol]: 432.63

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.07		Crippen Method
logp	4.618		Crippen Method
rinpol	2619.00		NIST Webbook
rinpol	2619.00		NIST Webbook
rinpol	2620.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R270923&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/50-745-9/GA20-ethyl-ester-TMS.pdf>

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