

GA118, MeTMS

Inchi: InChI=1S/C26H42O6Si2/c1-16-14-24-15-25(16,32-34(7,8)9)13-10-17(24)26-18(31-33(4,5)6)20-19-21-22-23-25
InchiKey: CZJKUGIUTGPWAY-IJVZLEIMSA-N
Formula: C26H42O6Si2
SMILES: C=C1CC23CC1(O[Si](C)(C)C)CCC2C12OC(=O)C(C)(CCC1O[Si](C)(C)C)C2C3C(=O)OC3
Mol. weight [g/mol]: 506.78

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.16		Crippen Method
logp	5.058		Crippen Method
rinpol	2686.00		NIST Webbook
rinpol	2690.00		NIST Webbook
rinpol	2689.00		NIST Webbook
rinpol	2690.00		NIST Webbook
rinpol	2685.00		NIST Webbook
rinpol	2686.00		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=R279539&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/69-706-2/GA118-MeTMS.pdf>

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