

GA4, MO-TMS

Inchi: InChI=1S/C26H42O5Si2/c1-16-11-13-25-15-17(16)9-10-18(25)26-14-12-19(30-32(3,4)5)
InchiKey: OKRPBAPBFGRULL-SWMWYWDKSA-N
Formula: C26H42O5Si2
SMILES: C=C1CCC23CC1CCC2C12CCC(O[Si](C)(C)C)(C)(C(=O)O1)C2C3C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 490.78

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.72		Crippen Method
logp	5.679		Crippen Method
rinpol	2604.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R604138&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/95-020-4/GA4-MO-TMS.pdf>

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