

GA68, MeTMSi

Other names: GA68, MeTMS
Inchi: InChI=1S/C26H40O6Si2/c1-15-16-10-11-17-25(14-16,21(15)32-34(7,8)9)19(22(27)29-3)
InchiKey: MYFUCFBJINCSHG-KSNFEXJQSA-N
Formula: C₂₆H₄₀O₆Si₂
SMILES: C=C1C2CCC3C45C=CC(O[Si](C)(C)C(C)(C(=O)O4)C5C(C(=O)OC)C3(C2)C1O[Si](C)
Mol. weight [g/mol]: 504.76

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.77		Crippen Method
logp	4.690		Crippen Method
rinpol	2695.00		NIST Webbook
rinpol	2681.00		NIST Webbook
rinpol	2682.00		NIST Webbook
rinpol	2694.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R79832&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/67-361-7/GA68-MeTMSi.pdf>

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