

GA30 isolactone, MeTMS

Inchi: InChI=1S/C26H40O6Si2/c1-15-13-25-14-16(15)17(31-33(4,5)6)12-18(25)26-11-10-19(32)
InchiKey: XQIUFDCAQUACFB-ZDKSYZROSA-N
Formula: C₂₆H₄₀O₆Si₂
SMILES: C=C1CC23CC1C(O[Si](C)(C)C)CC2C12C=CC(O[Si](C)(C)C)C(C)(C(=O)O1)C2C3C(=O)
Mol. weight [g/mol]: 504.76

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.77		Crippen Method
logp	4.690		Crippen Method
rinpol	2640.00		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R266018&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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/56-031-5/GA30-isolactone-MeTMS.pdf>

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