

Iso-GA3, MeTMSi

Inchi: InChI=1S/C26H40O6Si2/c1-16-14-24-15-25(16,32-34(7,8)9)12-10-17(24)26-13-11-18(31)
InchiKey: QJSHIGDRCGMRDL-FWGWZFZKRSA-N
Formula: C26H40O6Si2
SMILES: C=C1CC23CC1(O[Si](C)(C)C)CCC2C12C=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	-1.02		Crippen Method
logp	4.834		Crippen Method
rinpol	2659.00		NIST Webbook
rinpol	2659.00		NIST Webbook
rinpol	2637.00		NIST Webbook
rinpol	2638.00		NIST Webbook
rinpol	2642.00		NIST Webbook
rinpol	2659.00		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=R80102&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/22-147-4/Iso-GA3-MeTMSi.pdf>

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