

GA8-catabolite, MeTMS

Inchi: InChI=1S/C29H50O7Si3/c1-18-15-27-17-28(18,36-39(10,11)12)14-13-20(27)29-16-19(36)
InchiKey: URXALWQXBINWJP-QKOPFLJYSA-N
Formula: C29H50O7Si3
SMILES: C=C1CC23CC1(O[Si](C)(C)C)CCC2C12CC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(C)(C(=O)O)O1
Mol. weight [g/mol]: 594.96

Physical Properties

Property code	Value	Unit	Source
log10ws	0.33		Crippen Method
logp	5.888		Crippen Method
rinpol	2705.00		NIST Webbook
rinpol	2713.00		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=R299380&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/52-466-7/GA8-catabolite-MeTMS.pdf>

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