

GA50, MeTMSi

Inchi: InChI=1S/C29H50O7Si3/c1-17-14-28-15-18(17)13-19(34-37(4,5)6)22(28)29-16-20(35-38)
InchiKey: QVPGICUVUHIWGI-DZJDFXTKSA-N
Formula: C29H50O7Si3
SMILES: C=C1CC23CC1CC(O[Si](C)(C)C)C2C12CC(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	0.57		Crippen Method
logp	5.744		Crippen Method
rinpol	2847.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R79640&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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.cheméo.com/cid/14-591-0/GA50-MeTMSi.pdf>

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