

PGA1, BO-TMS, isomer # 1

Inchi: InChI=1S/C30H57NO4Si2/c1-9-11-15-18-27(34-36(3,4)5)23-21-26-22-24-29(31-33-25-12)
InchiKey: YOJSASACMPRYDX-CSHHMKSISA-N
Formula: C30H57NO4Si2
SMILES: CCCCCC(C=CC1C=CC(=NOCCCC)C1CCCCCCC(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 551.95

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.90		Crippen Method
logp	9.037		Crippen Method
rinpol	2768.00		NIST Webbook
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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=R581530&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/118-828-2/PGA1-BO-TMS-isomer-1.pdf>

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