

PGA1, MO-TMS, isomer # 1

Inchi: InChI=1S/C27H51NO4Si2/c1-9-10-13-16-24(31-33(3,4)5)21-19-23-20-22-26(28-30-2)25
InchiKey: ZDSXOMLVLPGWHE-SVCXTJLYSA-N
Formula: C27H51NO4Si2
SMILES: CCCCCC(C=CC1C=CC(=NOC)C1CCCCCCC(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 509.87

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.65		Crippen Method
logp	7.866		Crippen Method
rinpol	2542.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R581570&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/23-102-2/PGA1-MO-TMS-isomer-1.pdf>

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