

PGA2, MO-TMS, isomer # 1

Inchi: InChI=1S/C27H49NO4Si2/c1-9-10-13-16-24(31-33(3,4)5)21-19-23-20-22-26(28-30-2)25
InchiKey: RLZAGYMPBYGRFW-JMCNHHLISA-N
Formula: C27H49NO4Si2
SMILES: CCCCCC(C=CC1C=CC(=NOC)C1CC=CCCCC(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 507.85

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.50		Crippen Method
logp	7.642		Crippen Method
rinpol	2534.00		NIST Webbook
rinpol	2534.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R581634&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/47-829-0/PGA2-MO-TMS-isomer-1.pdf>

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