

PGB1, butyl oxime-TMS

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: ZAHHSCODEHQGOO-STELVPLLSA-N
Formula: C30H57NO4Si2
SMILES: CCCCCC(C=CC1=C(CCCCCC(=O)O[Si](C)(C)C)C(=NOCCCC)CC1)O[Si](C)(C)C
Mol. weight [g/mol]: 551.95

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.39		Crippen Method
logp	9.325		Crippen Method
rinpol	2943.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R581654&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/65-273-7/PGB1-butyl-oxime-TMS.pdf>

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