

Prosta-8(12),13-dien-1-oic acid, 9-(methoxyimino)-15-[(trimethylsilyl)oxy]-, trimethylsilyl ester

Other names:

ProB1 methyl oxime-TMS

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: ZGUGYUAUEGQMTR-LLYMUGNLSA-N

Formula: C27H51NO4Si2

SMILES: CCCCCC(C=CC1=C(CCCCCC(=O)O[Si](C)(C)C)C(=NOC)CC1)O[Si](C)(C)C

Mol. weight [g/mol]: 509.87

CAS: 72150-31-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.13		Crippen Method
logp	8.155		Crippen Method
rinpol	2696.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C72150313&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

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