

13,14-Dihydro-15-keto-PGF 2A, TMS

Inchi: InChI=1S/C29H58O5Si3/c1-11-12-15-18-24(30)21-22-26-25(19-16-13-14-17-20-29(31)32-28)/q3-5/p-1/s-
InchiKey: MSMSAAVJCYZXJI-UCQNIBCKSA-N
Formula: C₂₉H₅₈O₅Si₃
SMILES: CCCCCC(=O)CCC1C(O[Si](C)(C)C)CC(O[Si](C)(C)C)C1CC=CCCCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 571.02

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.92		Crippen Method
logp	8.487		Crippen Method
rinpol	2717.00		NIST Webbook
rinpol	2717.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R580700&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.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.chemeo.com/cid/123-206-6/13-14-Dihydro-15-keto-PGF-2A-TMS.pdf>

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