

Naloxone, bis(trimethylsilyl) ether

Inchi: InChI=1S/C25H37NO4Si2/c1-8-14-26-15-13-24-21-17-9-10-19(29-31(2,3)4)22(21)28-23(24)25H/t1,8,14,26,15,13,24,21,17,9,10,19,29,31,2,3,4,22,21,28,23,24,25/s1,8,14,26,15,13,24,21,17,9,10,19,29,31,2,3,4,22,21,28,23,24,25
InchiKey: TVMSEGLIEPBTNB-UHFFFAOYSA-N
Formula: C₂₅H₃₇NO₄Si₂
SMILES: C=CCN1CCC23c4c5ccc(O[Si](C)(C)C)c4OC2C(=O)CCC3(O[Si](C)(C)C)C1C5
Mol. weight [g/mol]: 471.74

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.24		Crippen Method
logp	4.669		Crippen Method
rinpol	2769.40		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U417209&Units=SI>

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/83-815-5/Naloxone-bis-trimethylsilyl-ether.pdf>

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