

Nalmefene, trimethylsilyl ether

Other names:	Nalmefene, tms derivative
Inchi:	InChI=1S/C24H33NO3Si/c1-15-9-10-24(26)19-13-17-7-8-18(28-29(2,3)4)21-20(17)23(24)
InchiKey:	HIFRSXPXRJAAFN-UHFFFAOYSA-N
Formula:	C ₂₄ H ₃₃ NO ₃ Si
SMILES:	C=C1CCC2(O)C3Cc4ccc(O[Si](C)(C)C)c5c4C2(CCN3CC2CC2)C1O5
Mol. weight [g/mol]:	411.61

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.32		Crippen Method
logp	4.021		Crippen Method
rinsol	2788.30		NIST Webbook
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Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333478&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
rinsol:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/11-704-7/Nalmefene-trimethylsilyl-ether.pdf>

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