Nalbuphine, O,O,O-tris(trimethylsilyl) deriv.

Other names:	Nalbuphine tris-O-TMS
	Nalbuphine, 3tms derivative
Inchi:	InChI=1S/C30H51NO4Si3/c1-36(2,3)33-23-14-13-22-19-25-30(35-38(7,8)9)16-15-24(34-
InchiKey:	MDKVPTBHJZRSKX-UHFFFAOYSA-N
Formula:	C30H51NO4Si3
SMILES:	C[Si](C)(C)Oc1ccc2c3c1OC1C(O[Si](C)(C)C)CCC4(O[Si](C)(C)C)C(C2)N(CC2CCC2)CC
Mol. weight [g/mol]:	573.99

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.10		Crippen Method
logp	6.934		Crippen Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U281193&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

Latest version available from:
https://www.chemeo.com/cid/98-919-4/Nalbuphine-O-O-O-tris-trimethylsilyl-deriv.pdf
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