

Butorphanol di-TMS derivative

Other names:	Butorphanol bis-O-TMS Butorphanol, 2tms derivative
Inchi:	InChI=1S/C27H45NO2Si2/c1-31(2,3)29-23-13-12-22-18-25-27(30-32(4,5)6)15-8-7-14-26
InchiKey:	WFWGEGWBULEAGY-UHFFFAOYSA-N
Formula:	C27H45NO2Si2
SMILES:	C[Si](C)(C)Oc1ccc2c(c1)C13CCCCC1(O[Si](C)(C)C)C(C2)N(CC1CCC1)CC3
Mol. weight [g/mol]:	471.82

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.89		Crippen Method
logp	6.733		Crippen Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U137237&Units=SI

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/86-245-5/Butorphanol-di-TMS-derivative.pdf>

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