

Quinine, trimethylsilyl ether

Other names:	Quinine, tms derivative
Inchi:	InChI=1S/C23H32N2O2Si/c1-6-16-15-25-12-10-17(16)13-22(25)23(27-28(3,4)5)19-9-11-
InchiKey:	UKECXMWGKYEZPW-UHFFFAOYSA-N
Formula:	C23H32N2O2Si
SMILES:	<chem>C=CC1CN2CCC1CC2C(O[Si](C)(C)C)c1ccnc2ccc(OC)cc12</chem>
Mol. weight [g/mol]:	396.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.01		Crippen Method
logp	5.032		Crippen Method
rinpol	2692.10		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352509&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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/11-329-4/Quinine-trimethylsilyl-ether.pdf>

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