Ibuprofen, tert-butyldimethylsilyl ester

Other names:	Ibuprofen, TBDMS
Inchi:	InChI=1S/C19H32O2Si/c1-14(2)13-16-9-11-17(12-10-16)15(3)18(20)21-22(7,8)19(4,5)6/h
InchiKey:	QMEKPXMERNLPJY-UHFFFAOYSA-N
Formula:	C19H32O2Si
SMILES:	CC(C)Cc1ccc(C(C)C(=O)O[Si](C)(C)C(C)(C)C)cc1
Mol. weight [g/mol]:	320.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.48		Crippen Method
logp	5.537		Crippen Method
rinpol	1876.50		NIST Webbook

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=U378440&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices