Tolmetin, TBDMS

Inchi: InChI=1S/C21H29NO3Si/c1-15-8-10-16(11-9-15)20(24)18-13-12-17(22(18)5)14-19(23)25
InchiKey: KEVJKOBQVLWWFP-UHFFFAOYSA-N
Formula: C21H29NO3Si
SMILES: Cc1ccc(C(=O)c2ccc(CC(=O)O[Si](C)(C)C(C)(C)C)n2C)cc1
Mol. weight [g/mol]: 371.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.42		Crippen Method
logp	4.655		Crippen Method
rinpol	2661.40		NIST Webbook
rinpol	2661.40		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R258730&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
rinpol: Non-polar retention indices