Kainic acid, N-isoBOC TBDMS

Inchi: InChI=1S/C24H45NO6Si2/c1-16(2)15-29-23(28)25-14-19(17(3)4)18(13-20(26)30-32(8,9)
InchiKey: XGPOXOGVFCKYQJ-KTVLMBSMSA-N
Formula: C24H45NO6Si2
SMILES: C=C(C)C1CN(C(=O)OCC(C)C)C(C(=O)O[Si](C)(C)C(C)(C)C)C1CC(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 499.79

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.24		Crippen Method
logp	5.588		Crippen Method
rinpol	2680.00		NIST Webbook
rinpol	2680.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R260545&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