

Kainic acid, TBDMS

Inchi: InChI=1S/C22H45NO4Si2/c1-15(2)17-14-23-19(20(25)27-29(11,12)22(6,7)8)16(17)13-18
InchiKey: GCBJQUPTUXLCHM-ZIFCJYIRSA-N
Formula: C22H45NO4Si2
SMILES: CC(C)C1CNC(C(=O)O[Si](C)(C)C(C)(C)C)C1CC(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 443.77

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.33		Crippen Method
logp	5.333		Crippen Method
rinpol	2562.00		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R564515&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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.cheméo.com/cid/25-258-8/Kainic-acid-TBDMS.pdf>

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