

3-Hydroxykynurenic acid, TMS

Inchi: InChI=1S/C19H31NO4Si3/c1-25(2,3)22-17-14-12-10-11-13-15(14)20-16(18(17)23-26(4,5)27-28)19-3
InchiKey: MYDHGOQGQGNWZHZ-UHFFFAOYSA-N
Formula: C19H31NO4Si3
SMILES: C[Si](C)(C)OC(=O)c1nc2ccccc2c(O[Si](C)(C)C)c1O[Si](C)(C)C
Mol. weight [g/mol]: 421.71

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.19		Crippen Method
logp	5.654		Crippen Method
rinpol	2377.00		NIST Webbook
rinpol	2377.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R400550&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.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.chemeo.com/cid/37-317-9/3-Hydroxykynurenic-acid-TMS.pdf>

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