

Kynurenic acid, tert-butyldimethylsilyl ether, tert-butyldimethylsilyl ester

Other names: tert-Butyl(dimethyl)silyl
Inchi: 4-pyrrolo[tert-butyl(dimethyl)silyl]oxymorphoquinoline-2-carboxylate
InchiKey: OVYHNSMEEINMQI-UHFFFAOYSA-N
Formula: C₂₂H₃₅NO₃Si₂
SMILES: CC(C)(C)[Si](C)(C)OC(=O)c1cc(O[Si](C)(C)C(C)(C)C)c2ccccc2n1
Mol. weight [g/mol]: 417.69
CAS: 959099-53-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.69		Crippen Method
logp	6.781		Crippen Method
rinpol	2554.60		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C959099537&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/120-260-9/Kynurenic-acid-tert-butyldimethylsilyl-ether-tert-butyldimethylsilyl-ester.pdf>

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