

Aspartic acid, MTH-TMS

Inchi: InChI=1S/C12H24N2O3SSi2/c1-14-11(17-20(5,6)7)9(13-12(14)18)8-10(15)16-19(2,3)4/h
InchiKey: QIBGKCAFXJWNKO-UHFFFAOYSA-N
Formula: C12H24N2O3SSi2
SMILES: Cn1c(O[Si](C)(C)C)c(CC(=O)O[Si](C)(C)C)[nH]c1=S
Mol. weight [g/mol]: 332.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.81		Crippen Method
logp	2.735		Crippen Method
rinpol	1896.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R525392&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

Latest version available from:

<https://www.chemeo.com/cid/54-352-1/Aspartic-acid-MTH-TMS.pdf>

Generated by Cheméo on 2025-12-05 22:44:07.548204246 +0000 UTC m=+4722845.078244899.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.