

Glutamine, MTH-TMS

Inchi: InChI=1S/C13H27N3O2SSi2/c1-16-12(18-21(5,6)7)10(14-13(16)19)8-9-11(17)15-20(2,3)
InchiKey: MCLCKJTUSKPGEP-UHFFFAOYSA-N
Formula: C13H27N3O2SSi2
SMILES: Cn1c(O[Si](C)(C)C)c(CCC(=O)N[Si](C)(C)C)[nH]c1=S
Mol. weight [g/mol]: 345.61

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.33		Crippen Method
logp	2.698		Crippen Method
rinpol	2154.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R525421&Units=SI>

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/34-355-0/Glutamine-MTH-TMS.pdf>

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