

B-Ala, TMS, # 2

Inchi: InChI=1S/C9H23NO2Si2/c1-13(2,3)10-8-7-9(11)12-14(4,5)6/h10H,7-8H2,1-6H3
InchiKey: WRNXABBYSLTNAT-UHFFFAOYSA-N
Formula: C9H23NO2Si2
SMILES: C[Si](C)(C)NCCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 233.46

Physical Properties

Property code	Value	Unit	Source
log10ws	2.26		Crippen Method
logp	2.179		Crippen Method
rinpol	1438.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R485833&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.chemeo.com/cid/117-218-0/B-Ala-TMS-2.pdf>

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