

(5S,6S)-6-tert-Butyldimethylsilyloxy-5-hydroxyazepane-2-one

Inchi: InChI=1S/C12H25NO3Si/c1-12(2,3)17(4,5)16-10-8-13-11(15)7-6-9(10)14/h9-10,14H,6-8H
InchiKey: VEFKXRYRNUCBQS-NXEZZACHSA-N
Formula: C12H25NO3Si
SMILES: CC(C)(C)[Si](C)(C)OC1CNC(=O)CCC1O
Mol. weight [g/mol]: 259.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.33		Crippen Method
logp	1.648		Crippen Method
rinpol	1971.00		NIST Webbook
rinpol	1971.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R500353&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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