

Propanoic acid, 3-[(tert-butyl dimethylsilyl)oxy]-, tert-butyl dimethylsilyl ester

Other names: 3-Hydroxypropionic acid, diTBDMS
3-Hydroxypropionic acid, TBDMS
Hydracrylic acid, 2tdms derivative

Inchi: InChI=1S/C15H34O3Si2/c1-14(2,3)19(7,8)17-12-11-13(16)18-20(9,10)15(4,5)6/h11-12H

InchiKey: GTADNJPZLIFKDX-UHFFFAOYSA-N

Formula: C15H34O3Si2

SMILES: CC(C)(C)[Si](C)(C)OCCC(=O)O[Si](C)(C)C(C)(C)C

Mol. weight [g/mol]: 318.60

CAS: 82112-30-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.15		Crippen Method
logp	4.947		Crippen Method
rinpol	1580.00		NIST Webbook
rinpol	1578.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: https://www.chemo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C82112309&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.chemo.com/cid/59-423-7/Propanoic-acid-3-tert-butyl-dimethylsilyl-oxy-tert-butyl-dimethylsilyl-ester.pdf>

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