

(R)-3-Hydroxybutyric acid, trimethylsilyl ether, trimethylsilyl ester

Other names:	Trimethylsilyl (3R)-3-[(trimethylsilyl)oxy]butanoate (R)-3-hydroxybutyric acid, 2tms derivative
Inchi:	InChI=1S/C10H24O3Si2/c1-9(12-14(2,3)4)8-10(11)13-15(5,6)7/h9H,8H2,1-7H3
InchiKey:	YWRIHOYCAHATJN-UHFFFAOYSA-N
Formula:	C10H24O3Si2
SMILES:	CC(CC(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]:	248.47

Physical Properties

Property code	Value	Unit	Source
log10ws	1.83		Crippen Method
logp	2.995		Crippen Method
rinpol	1147.90		NIST Webbook

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=U332958&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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