

Butane, 1,2,3-tris(trimethylsiloxy)-

Other names:	1,2,3-Butanetriol, 3 TMS
Inchi:	InChI=1S/C13H34O3Si3/c1-12(15-18(5,6)7)13(16-19(8,9)10)11-14-17(2,3)4/h12-13H,11
InchiKey:	YXTPRNAJOICBLA-UHFFFAOYSA-N
Formula:	C13H34O3Si3
SMILES:	CC(O[Si](C)(C)C)C(CO[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]:	322.66
CAS:	33581-76-9

Physical Properties

Property code	Value	Unit	Source
log10ws	3.10		Crippen Method
logp	4.298		Crippen Method
rinpola	1285.70		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=C33581769&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/112-934-0/Butane-1-2-3-tris-trimethylsiloxy.pdf>

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