

Butanoic acid, trimethylsilyl ester

Other names:	Butyric acid, trimethylsilyl ester Butyroxyltrimethylsilane Butyric acid, tms derivative
Inchi:	InChI=1S/C7H16O2Si/c1-5-6-7(8)9-10(2,3)4/h5-6H2,1-4H3
InchiKey:	YOXUKTJZXUYZMV-UHFFFAOYSA-N
Formula:	C7H16O2Si
SMILES:	CCCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	160.29
CAS:	16844-99-8

Physical Properties

Property code	Value	Unit	Source
log10ws	0.33		Crippen Method
logp	2.165		Crippen Method
rinpol	881.50		NIST Webbook
rinpol	891.00		NIST Webbook
rinpol	883.00		NIST Webbook
ripol	1025.00		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=C16844998&Units=SI

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/40-661-3/Butanoic-acid-trimethylsilyl-ester.pdf>

Generated by Cheméo on 2024-04-20 14:33:49.754059261 +0000 UTC m=+15912878.674636576.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.