

Butyric acid, tert-butyldimethylsilyl ester

Other names:	tert-Butyl(dimethyl)silyl butyrate Butanoic acid, TBDMS Butanoic acid, DMTBS Butyric acid, TBDMS Butyric acid, tbdms derivative
Inchi:	InChI=1S/C10H22O2Si/c1-7-8-9(11)12-13(5,6)10(2,3)4/h7-8H2,1-6H3
InchiKey:	LYRXFUFOQFNGPJ-UHFFFAOYSA-N
Formula:	C10H22O2Si
SMILES:	CCCC(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	202.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.92		Crippen Method
logp	3.335		Crippen Method
rinpol	1098.90		NIST Webbook
rinpol	1097.00		NIST Webbook
rinpol	1074.00		NIST Webbook
rinpol	1103.00		NIST Webbook
rinpol	1097.00		NIST Webbook
rinpol	1098.00		NIST Webbook
ripol	1200.00		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=U333136&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

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