

Propanoic acid, t-butyldimethylsilyl ester

Other names:	Propanoic acid, DMTBS Propanoic acid, TBDMS Propanoic acid, tert-butyldimethylsilyl ester Propionic acid, TBDMS tert-Butyl(dimethyl)silyl propionate Propanoic acid, tbdms derivative
Inchi:	InChI=1S/C9H20O2Si/c1-7-8(10)11-12(5,6)9(2,3)4/h7H2,1-6H3
InchiKey:	WNORCYXNCTYGSE-UHFFFAOYSA-N
Formula:	C9H20O2Si
SMILES:	CCC(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	188.34
CAS:	111864-20-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.50		Crippen Method
logp	2.945		Crippen Method
rinpol	1017.20		NIST Webbook
rinpol	1015.00		NIST Webbook
rinpol	1017.00		NIST Webbook
rinpol	990.00		NIST Webbook
rinpol	1019.00		NIST Webbook
rinpol	1017.20		NIST Webbook
rinpol	1015.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C111864201&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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