Pentanoic acid, tert-butyldimethylsilyl ester

Other names:	Pentanoic acid, DMTBS
	Pentanoic acid, TBDMS
	Valeric acid, DMTBS
	Valeric acid, TBDMS
	tert-Butyl(dimethyl)silyl pentanoate
	Pentanoic acid, tbdms derivative
Inchi:	InChI=1S/C11H24O2Si/c1-7-8-9-10(12)13-14(5,6)11(2,3)4/h7-9H2,1-6H3
InchiKey:	NZFSRCPLEXEGDZ-UHFFFAOYSA-N
Formula:	C11H24O2Si
SMILES:	CCCCC(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	216.39
CAS:	104256-46-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.34		Crippen Method
logp	3.725		Crippen Method
rinpol	1198.10		NIST Webbook
rinpol	1184.00		NIST Webbook
rinpol	1195.00		NIST Webbook
rinpol	1196.00		NIST Webbook
rinpol	1198.10		NIST Webbook
rinpol	1195.00		NIST Webbook
rinpol	1196.00		NIST Webbook
rinpol	1174.00		NIST Webbook
ripol	1294.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C104256464&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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