Pentanoic acid, trimethylsilyl ester

Other names:	Valeric acid, trimethylsilyl ester
	Trimethylsilyl pentanoate
	Pentanoic acid, tms derivative
Inchi:	InChI=1S/C8H18O2Si/c1-5-6-7-8(9)10-11(2,3)4/h5-7H2,1-4H3
InchiKey:	KBBNGLHDTQGESG-UHFFFAOYSA-N
Formula:	C8H18O2Si
SMILES:	CCCCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	174.31
CAS:	26429-16-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.08		Crippen Method
logp	2.555		Crippen Method
rinpol	974.00		NIST Webbook
rinpol	973.10		NIST Webbook
rinpol	975.00		NIST Webbook
rinpol	977.00		NIST Webbook
rinpol	1015.00		NIST Webbook
ripol	1123.00		NIST Webbook
ripol	1123.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26429163&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

ripol: Polar retention indices