

Heptanoic acid, trimethylsilyl ester

Other names:	Heptanoic acid, TMS Heptanoic acid, TMS ester Heptanoic acid, tms derivative
Inchi:	InChI=1S/C10H22O2Si/c1-5-6-7-8-9-10(11)12-13(2,3)4/h5-9H2,1-4H3
InchiKey:	AMUGRUMFZAKWNM-UHFFFAOYSA-N
Formula:	C10H22O2Si
SMILES:	CCCCCCC(=O)O[Si](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	1162.00		NIST Webbook
rinpol	1168.70		NIST Webbook
rinpol	1166.00		NIST Webbook
rinpol	1162.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1168.70		NIST Webbook
rinpol	1171.20		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333733&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
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logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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