

Hexanoic acid, trimethylsilyl ester

Other names:	Caproic acid, trimethylsilyl ester Hexanoic acid, TMS Hexanoic acid, tms derivative
Inchi:	InChI=1S/C9H20O2Si/c1-5-6-7-8-9(10)11-12(2,3)4/h5-8H2,1-4H3
InchiKey:	CYXNJMDACJPPRR-UHFFFAOYSA-N
Formula:	C9H20O2Si
SMILES:	CCCCCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	188.34
CAS:	14246-15-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.50		Crippen Method
logp	2.945		Crippen Method
rinpol	1063.00		NIST Webbook
rinpol	1074.00		NIST Webbook
rinpol	1063.00		NIST Webbook
rinpol	1071.00		NIST Webbook
rinpol	1068.60		NIST Webbook
rinpol	1073.30		NIST Webbook
rinpol	1071.00		NIST Webbook
rinpol	1069.00		NIST Webbook
rinpol	1063.00		NIST Webbook
rinpol	1074.00		NIST Webbook
rinpol	1074.00		NIST Webbook
rinpol	1074.00		NIST Webbook
rinpol	1074.00		NIST Webbook
rinpol	1074.00		NIST Webbook
rinpol	1071.00		NIST Webbook
rinpol	1064.00		NIST Webbook
rinpol	1074.00		NIST Webbook
rinpol	1071.00		NIST Webbook
rinpol	1063.00		NIST Webbook
rinpol	1073.00		NIST Webbook
ripol	1200.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C14246152&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/15-892-5/Hexanoic-acid-trimethylsilyl-ester.pdf>

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