

Pentanoic acid, 2-propyl, trimethylsilyl ester

Other names:	Heptane-4-carboxylic acid, TMS
Inchi:	InChI=1S/C11H24O2Si/c1-6-8-10(9-7-2)11(12)13-14(3,4)5/h10H,6-9H2,1-5H3
InchiKey:	KAWLRPDXEKBP RS-UHFFFAOYSA-N
Formula:	C11H24O2Si
SMILES:	CCCC(CCC)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	216.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.28		Cheméo Relay (1.0)
logp	3.581		Crippen Method
rinpol	1156.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1147.00		NIST Webbook
rinpol	1141.00		NIST Webbook
rinpol	1150.00		NIST Webbook
rinpol	1147.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1150.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1141.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1151.00		NIST Webbook
tb	460.35	K	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U79510&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

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

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<https://www.cheméo.com/cid/98-676-4/Pentanoic-acid-2-propyl-trimethylsilyl-ester.pdf>

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