

Dipropylacetic acid, 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:	KAWLRPDXEKBPRS-UHFFFAOYSA-N
Formula:	C11H24O2Si
SMILES:	CCCC(CCC)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	216.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.10		Crippen Method
logp	3.581		Crippen Method
rinpola	1150.00		NIST Webbook
rinpola	1151.00		NIST Webbook
rinpola	1141.00		NIST Webbook

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

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/98-676-4/Dipropylacetic-acid-trimethylsilyl-ester.pdf>

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