

Cyclohexanecarboxylic acid, trimethylsilyl ester

Other names:	Cyclohexanecarboxylic acid, tms derivative
Inchi:	InChI=1S/C10H20O2Si/c1-13(2,3)12-10(11)9-7-5-4-6-8-9/h9H,4-8H2,1-3H3
InchiKey:	PYJUBHQOZUNCIC-UHFFFAOYSA-N
Formula:	C10H20O2Si
SMILES:	C[Si](C)(C)OC(=O)C1CCCCC1
Mol. weight [g/mol]:	200.35
CAS:	69435-89-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.57		Crippen Method
logp	2.945		Crippen Method
rinpola	1188.00		NIST Webbook
rinpola	1188.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C69435898&Units=SI

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/91-802-0/Cyclohexanecarboxylic-acid-trimethylsilyl-ester.pdf>

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