

Hexanoic acid, bromomethyldimethylsilyl ester

Inchi:	InChI=1S/C9H19BrO2Si/c1-4-5-6-7-9(11)12-13(2,3)8-10/h4-8H2,1-3H3
InchiKey:	GDDDIADSKDSQK-UHFFFAOYSA-N
Formula:	C9H19BrO2Si
SMILES:	CCCCC(=O)O[Si](C)(C)CBr
Mol. weight [g/mol]:	267.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.02		Crippen Method
logp	3.249		Crippen Method
rinpol	1365.00		NIST Webbook
rinpol	1365.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375590&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/113-207-6/Hexanoic-acid-bromomethyldimethylsilyl-ester.pdf>

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