

Butyric acid, dimethyl(3,3,3-trifluoropropyl)silyl ester

Inchi: InChI=1S/C9H17F3O2Si/c1-4-5-8(13)14-15(2,3)7-6-9(10,11)12/h4-7H2,1-3H3
InchiKey: SKNRKYZJVPBETQ-UHFFFAOYSA-N
Formula: C9H17F3O2Si
SMILES: CCCC(=O)O[Si](C)(C)CC(F)(F)F
Mol. weight [g/mol]: 242.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.17		Crippen Method
logp	3.487		Crippen Method
rinpol	1020.00		NIST Webbook
rinpol	1020.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U375601&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

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<https://www.cheméo.com/cid/81-415-1/Butyric-acid-dimethyl-3-3-3-trifluoropropyl-silyl-ester.pdf>

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