

Butanal, TMS (possibly, MSTFA-adduct)

Inchi: InChI=1S/C10H20F3NO2Si/c1-6-7-8(16-17(3,4)5)14(2)9(15)10(11,12)13/h8H,6-7H2,1-5H
InchiKey: GGMHCPMOQDXVTI-UHFFFAOYSA-N
Formula: C10H20F3NO2Si
SMILES: CCCC(O[Si](C)(C)C)N(C)C(=O)C(F)(F)F
Mol. weight [g/mol]: 271.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.76		Crippen Method
logp	2.985		Crippen Method
rinpol	1375.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R631313&Units=SI>

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/76-847-8/Butanal-TMS-possibly-MSTFA-adduct.pdf>

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