

2-Ketobutyric acid, tert-butyldimethylsilyl ester

Other names:	2-Ketobutyric acid, tbdms derivative
Inchi:	InChI=1S/C10H20O3Si/c1-7-8(11)9(12)13-14(5,6)10(2,3)4/h7H2,1-6H3
InchiKey:	OUBLLMRWJIKKGY-UHFFFAOYSA-N
Formula:	C10H20O3Si
SMILES:	CCC(=O)C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	216.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.20		Crippen Method
logp	2.514		Crippen Method
rinpol	1196.30		NIST Webbook
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Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333752&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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.chemeo.com/cid/57-678-7/2-Ketobutyric-acid-tert-butyldimethylsilyl-ester.pdf>

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