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
rinpol	1196.30		NIST Webbook

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