

Glycine, N-(3-methyl-1-oxobutyl)-, trimethylsilyl ester

Other names:

Isovaleroglycine, trimethylsilyl ester
N-Isovalerylglycine, trimethylsilyl ester
Acetic acid, isopentanoylamino, oxime, mono-TMS
Glycine, N-isopentanoyl, TMS
Glycine, N-isovaleroyl, mono-TMS
Glycine, N-isovaleroyl, TMS ester
Isovalerylglycine, mono-TMS
N-isovaleroylglycine, tms derivative

Inchi:

InChI=1S/C10H21NO3Si/c1-8(2)6-9(12)11-7-10(13)14-15(3,4)5/h8H,6-7H2,1-5H3,(H,11,

InchiKey:

LGRAJBIRLFSLRM-UHFFFAOYSA-N

Formula:

C10H21NO3Si

SMILES:

CC(C)CC(=O)NCC(=O)O[Si](C)(C)C

Mol. weight [g/mol]:

231.36

CAS:

55494-00-3

Physical Properties

Property code	Value	Unit	Source
log10ws	0.36		Crippen Method
logp	1.527		Crippen Method
rinpol	1464.00		NIST Webbook
rinpol	1495.00		NIST Webbook
rinpol	1502.00		NIST Webbook
rinpol	1462.00		NIST Webbook
rinpol	1502.00		NIST Webbook
rinpol	1488.00		NIST Webbook
rinpol	1464.00		NIST Webbook
rinpol	1488.70		NIST Webbook
rinpol	1505.00		NIST Webbook
rinpol	1464.00		NIST Webbook
rinpol	1501.00		NIST Webbook
rinpol	1488.70		NIST Webbook
rinpol	1501.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C55494003&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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