Butanoic acid, 4,4'-dithiobis[2-[(trimethylsilyl)amino]-, bis(trimethylsilyl) ester, [S-(R*,R*)]-

Other names: L-Homocystine, N,N'-bis(trimethylsilyl)-, bis(trimethylsilyl) ester
L-homocystine, [s-(r*,r*)]-, 4tms derivative

Inchi: InChI=1S/C20H48N2O4S2Si4/c1-29(2,3)21-17(19(23)25-31(7,8)9)13-15-27-28-16-14-18

InchiKey: VVODJOVRLCDBOE-UHFFFAOYSA-N

Formula: C20H48N2O4S2Si4

SMILES: C[Si](C)(C)NC(CCSSCCC(N[Si](C)(C)C)C(=O)O[Si](C)(C)C)C(=O)O[Si](C)(C)C

Mol. weight [g/mol]: 557.08

CAS: 69688-45-5

Physical Properties

Property code	Value	Unit	Source
log10ws	2.52		Crippen Method
logp	5.490		Crippen Method
rinpol	2512.40		NIST Webbook
rinpol	2577.00		NIST Webbook
rinpol	2577.00		NIST Webbook
rinpol	2512.40		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C69688455&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

Latest version available from: