

Benzenebutanoic acid, «gamma»-oxo-«alpha»,2-bis[(trimethylsilyl)amino] trimethylsilyl ester

Other names:

Kynurenine, tri-TMS II

Kynurenine, 3tms derivative

Inchi: InChI=1S/C19H36N2O3Si3/c1-25(2,3)20-16-13-11-10-12-15(16)18(22)14-17(21-26(4,5)6)
InchiKey: MGAWBUDKVLGSOC-UHFFFAOYSA-N
Formula: C19H36N2O3Si3
SMILES: C[Si](C)(C)Nc1cccc1C(=O)CC(N[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 424.76
CAS: 72088-03-0

Physical Properties

Property code	Value	Unit	Source
log10ws	1.36		Crippen Method
logp	4.677		Crippen Method
rinpol	2183.90		NIST Webbook
rinpol	2183.90		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C72088030&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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