

Histidine, ethoxycarbonylated, TBDMS

Inchi: InChI=1S/C18H31N3O6Si/c1-8-25-16(23)20-14(15(22)27-28(6,7)18(3,4)5)10-13-11-21(12)
InchiKey: CHEOLGUBFQGKRO-UHFFFAOYSA-N
Formula: C18H31N3O6Si
SMILES: CCOC(=O)NC(Cc1cn(C(=O)OCC)cn1)C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 413.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.41		Crippen Method
logp	3.093		Crippen Method
rinpol	2504.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R564411&Units=SI>

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/26-488-2/Histidine-ethoxycarbonylated-TBDMS.pdf>

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