

Pyroglutamic acid, TMS

Other names:

Pyroglutamic acid, di-TMS
Pyroglutamic acid, bis-TMS
PYROGLUTAMIC diTMS
Pyroglytamic acid, TMS

Inchi: InChI=1S/C11H23NO3Si2/c1-16(2,3)14-10-8-7-9(12-10)11(13)15-17(4,5)6/h9H,7-8H2,1-**InchiKey:** RGRQCHDQMZLOLU-UHFFFAOYSA-N**Formula:** C11H23NO3Si2**SMILES:** C[Si](C)(C)OC(=O)C1CCC(O[Si](C)(C)C)=N1**Mol. weight [g/mol]:** 273.48

Physical Properties

Property code	Value	Unit	Source
log10ws	1.86		Crippen Method
logp	2.777		Crippen Method
rinpol	1536.00		NIST Webbook
rinpol	1523.00		NIST Webbook
rinpol	1508.00		NIST Webbook
rinpol	1505.00		NIST Webbook
rinpol	1536.00		NIST Webbook
rinpol	1509.00		NIST Webbook
rinpol	1536.00		NIST Webbook
rinpol	1540.00		NIST Webbook
rinpol	1507.00		NIST Webbook
rinpol	1510.00		NIST Webbook
rinpol	1507.00		NIST Webbook
rinpol	1529.00		NIST Webbook
rinpol	1517.00		NIST Webbook
rinpol	1529.00		NIST Webbook
rinpol	1510.00		NIST Webbook
rinpol	1540.00		NIST Webbook
rinpol	1509.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R44875&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:

<https://www.chemeo.com/cid/116-887-9/Pyroglutamic-acid-TMS.pdf>

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