Furoylglycine, trimethylsilyl ester

Other names:	Furoyl glycine, mono-TMS
	N-2-Furoylglycine, trimethylsilyl ester
	N-Furoylglycine, mono-TMS
	Furoylglycine, tms derivative
Inchi:	InChI=1S/C10H15NO4Si/c1-16(2,3)15-9(12)7-11-10(13)8-5-4-6-14-8/h4-6H,7H2,1-3H3,(
InchiKey:	LFHIJMKOVQHKJV-UHFFFAOYSA-N
Formula:	C10H15NO4Si
SMILES:	C[Si](C)(C)OC(=O)CNC(=O)c1ccco1
Mol. weight [g/mol]:	241.32
CAS:	71428-92-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.14		Crippen Method
logp	1.387		Crippen Method
rinpol	1664.00		NIST Webbook
rinpol	1617.00		NIST Webbook
rinpol	1617.00		NIST Webbook
rinpol	1662.10		NIST Webbook
rinpol	1656.00		NIST Webbook
rinpol	1662.10		NIST Webbook
rinpol	1664.00		NIST Webbook
rinpol	1656.00		NIST Webbook
rinpol	1662.40		NIST Webbook
rinpol	1617.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C71428927&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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