Glycine, N-(2-furanylcarbonyl)-, methyl ester

Other names:	Glycine, N-2-furoyl-, methyl ester
	Methyl N-2-furoylglycinate
	Methyl (2-furoylamino)acetate
	N-(2-Furoyl)glycine, methyl ester
	[(Furan-2-carbonyl)-amino]-acetic acid methyl ester
Inchi:	InChI=1S/C8H9NO4/c1-12-7(10)5-9-8(11)6-3-2-4-13-6/h2-4H,5H2,1H3,(H,9,11)
InchiKey:	MPRFBNLQEYNYQK-UHFFFAOYSA-N
Formula:	C8H9NO4
SMILES:	COC(=O)CNC(=O)c1ccco1
Mol. weight [g/mol]:	183.16
CAS:	13290-00-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.25		Crippen Method
logp	0.182		Crippen Method
mcvol	128.980	ml/mol	McGowan Method
rinpol	1522.20		NIST Webbook
rinpol	1523.60		NIST Webbook
rinpol	1471.00		NIST Webbook
rinpol	1471.00		NIST Webbook
rinpol	1471.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13290001&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices