

Glycine, n-2-imidazolin-2-yl-

Inchi:	InChI=1S/C5H9N3O2/c9-4(10)3-8-5-6-1-2-7-5/h1-3H2,(H,9,10)(H2,6,7,8)
InchiKey:	FITFYSPDBODJFN-UHFFFAOYSA-N
Formula:	C5H9N3O2
SMILES:	O=C([O-])CNC1=[NH+]CCN1
Mol. weight [g/mol]:	143.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.74		Crippen Method
logp	-4.634		Crippen Method
mcvol	103.530	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6006896&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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<https://www.chemeo.com/cid/41-899-9/Glycine-n-2-imidazolin-2-yl.pdf>

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