

# Pyrrolidine, 1-[(4-amino-1,2,5-thiadiazol-3-yl)carbonyl]-

Inchi:	InChI=1S/C7H10N4OS/c8-6-5(9-13-10-6)7(12)11-3-1-2-4-11/h1-4H2,(H2,8,10)
InchiKey:	KPCJLKMPVNIDIE-UHFFFAOYSA-N
Formula:	C7H10N4OS
SMILES:	Nc1nsnc1C(=O)N1CCCC1
Mol. weight [g/mol]:	198.25
CAS:	116374-00-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.27		Crippen Method
logp	0.356		Crippen Method
mcvol	137.010	ml/mol	McGowan Method

## Sources

Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C116374006&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116374006&amp;Units=SI</a>

## Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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