

# Urea, 1-methyl-1-nitroso-3-[(1,2,3,4-tetrahydro-2,4-dioxo

Inchi:	InChI=1S/C7H9N5O4/c1-12(11-16)7(15)9-3-4-2-8-6(14)10-5(4)13/h2H,3H2,1H3,(H,9,15)
InchiKey:	WPOPXYFSRHLARA-UHFFFAOYSA-N
Formula:	C7H9N5O4
SMILES:	CN(N=O)C(=O)NCc1c[nH]c(=O)[nH]c1=O
Mol. weight [g/mol]:	227.18
CAS:	89854-42-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.17		Crippen Method
logp	-2.078		Crippen Method
mcvol	150.510	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=C89854422&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C89854422&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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