

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

Inchi:	InChI=1S/C6H7N5O4/c1-11(10-15)6(14)8-3-2-7-5(13)9-4(3)12/h2H,1H3,(H,8,14)(H2,7,9,
InchiKey:	ZLMJEQGWFPWXSL-UHFFFAOYSA-N
Formula:	C6H7N5O4
SMILES:	CN(N=O)C(=O)Nc1c[nH]c(=O)[nH]c1=O
Mol. weight [g/mol]:	213.15
CAS:	58494-42-1

Physical Properties

Property code	Value	Unit	Source
log10ws	0.31		Crippen Method
logp	-1.756		Crippen Method
mcvol	136.420	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C58494421&Units=SI

Legend

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

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