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: 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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C89854422&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume