

Urea, 1-methyl-1-nitroso-3-(8-quinoly)-

Inchi:	InChI=1S/C11H10N4O2/c1-15(14-17)11(16)13-9-6-2-4-8-5-3-7-12-10(8)9/h2-7H,1H3,(H,
InchiKey:	DMUFDIMTYBEPHW-UHFFFAOYSA-N
Formula:	C11H10N4O2
SMILES:	CN(N=O)C(O)=Nc1cccc2cccnc12
Mol. weight [g/mol]:	230.22
CAS:	91091-63-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.68		Crippen Method
logp	2.393		Crippen Method
mcvol	165.690	ml/mol	McGowan Method

Sources

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=C91091633&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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/83-510-3/Urea-1-methyl-1-nitroso-3-8-quinolyl.pdf>

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