

2-Oxazolanone, 3-methyleneamino-

Inchi: InChI=1S/C4H6N2O2/c1-5-6-2-3-8-4(6)7/h1-3H2
InchiKey: CLFLNVLCRRFNQV-UHFFFAOYSA-N
Formula: C4H6N2O2
SMILES: C=NN1CCOC1=O
Mol. weight [g/mol]: 114.10
CAS: 10020-75-4

Physical Properties

Property code	Value	Unit	Source
log10ws	0.04		Crippen Method
logp	0.054		Crippen Method
mcvol	79.460	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C10020754&Units=SI>
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>

Legend

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

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