Uracil, 6-amino-1,3-dimethyl-5-nitroso-

Other names: 6-amino-1,3-dimethyl-5-nitrosouracil
Inchi: InChI=1S/C6H8N4O3/c1-9-4(7)3(8-13)5(11)10(2)6(9)12/h7H2,1-2H3
InchiKey: MGBDANYXBKROBW-UHFFFAOYSA-N
Formula: C6H8N4O3
SMILES: Cn1c(N)c(N=O)c(=O)n(C)c1=O
Mol. weight [g/mol]: 184.15
CAS: 6632-68-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.29		Crippen Method
logp	-0.936		Crippen Method
mcvol	124.870	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=C6632684&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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