

Urea, 1-(2-hydroxyethyl)-1-nitroso-3-(1,2,3,4-tetrahydro-

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|----------------------|--|
| Inchi: | InChI=1S/C7H9N5O5/c13-2-1-12(11-17)7(16)9-4-3-8-6(15)10-5(4)14/h3,13H,1-2H2,(H,9 |
| InchiKey: | IDSUPEKZVIGOGK-UHFFFAOYSA-N |
| Formula: | C7H9N5O5 |
| SMILES: | O=NN(CCO)C(=O)Nc1c[nH]c(=O)[nH]c1=O |
| Mol. weight [g/mol]: | 243.18 |
| CAS: | 89854-43-3 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | 0.63 | | Crippen Method |
| logp | -2.393 | | Crippen Method |
| mcvol | 156.380 | ml/mol | McGowan Method |

Sources

| | |
|-----------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C89854433&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307I |
| 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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