

3-Amino-1H-quinazoline-2,4-dione

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|-----------------------------|---|
| Inchi: | InChI=1S/C8H7N3O2/c9-11-7(12)5-3-1-2-4-6(5)10-8(11)13/h1-4H,9H2,(H,10,13) |
| InchiKey: | NMGODFWGUBLTTA-UHFFFAOYSA-N |
| Formula: | C8H7N3O2 |
| SMILES: | Nn1c(=O)[nH]c2ccccc2c1=O |
| Mol. weight [g/mol]: | 177.16 |
| CAS: | 30386-01-7 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -0.43 | | Crippen Method |
| logp | -1.078 | | Crippen Method |
| mcvol | 122.040 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|---|
| 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 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C30386017&Units=SI |

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/16-949-1/3-Amino-1H-quinazoline-2-4-dione.pdf>

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