

# benzoyleneurea

**Inchi:** InChI=1S/C8H6N2O2/c11-7-5-3-1-2-4-6(5)9-8(12)10-7/h1-4H,(H2,9,10,11,12)  
**InchiKey:** SDQJTWBNWQABLE-UHFFFAOYSA-N  
**Formula:** C8H6N2O2  
**SMILES:** O=c1[nH]c(=O)c2ccccc2[nH]1  
**Mol. weight [g/mol]:** 162.15

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.56		Crippen Method
logp	-0.747		Crippen Method
mcvol	112.060	ml/mol	McGowan Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	128.30 ± 3.00	kJ/mol	298.15	Energetics of Quinazoline-2,4(1H,3H)-dione: An Experimental and Computational Study

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**Energetics of Quinazoline-2,4(1H,3H)-dione: An Experimental and Computational Study:** <https://www.doi.org/10.1021/je2004929>

# Legend

<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume

Latest version available from:

<https://www.cheméo.com/cid/110-469-9/benzoyleneurea.pdf>

Generated by Cheméo on 2024-04-29 06:14:20.951242884 +0000 UTC m=+16660509.871820199.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.