

# 5-Iodocytosine

|                      |                                                                                                                                                                            |
|----------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | Cytosine, 5-iodo-<br>4-amino-5-iodopyrimidinone<br>4-Amino-5-iodo-2(1H)-pyrimidinone<br>2(1H)-Pyrimidinone, 4-amino-5-iodo-<br>5-Iodocytosine (4-amino-5-iodopyrimidinone) |
| Inchi:               | InChI=1S/C4H4IN3O/c5-2-1-7-4(9)8-3(2)6/h1H,(H3,6,7,8,9)                                                                                                                    |
| InchiKey:            | UFVWJVMULFOMC-UHFFFAOYSA-N                                                                                                                                                 |
| Formula:             | C4H4IN3O                                                                                                                                                                   |
| SMILES:              | <chem>N=c1[nH]c(O)ncc1I</chem>                                                                                                                                             |
| Mol. weight [g/mol]: | 237.00                                                                                                                                                                     |
| CAS:                 | 1122-44-7                                                                                                                                                                  |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -2.15   |        | Crippen Method |
| logp          | -0.283  |        | Crippen Method |
| mcvol         | 105.090 | ml/mol | McGowan Method |

## Temperature Dependent Properties

| Property code | Value         | Unit   | Temperature [K] | Source       |
|---------------|---------------|--------|-----------------|--------------|
| hsubt         | 144.00 ± 1.50 | kJ/mol | 438.00          | NIST Webbook |

## Sources

|                 |                                                                                                                                             |
|-----------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>                                   |
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                           |
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                       |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1122447&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1122447&amp;Units=SI</a> |

# Legend

|                 |                                                |
|-----------------|------------------------------------------------|
| <b>hsubt:</b>   | Enthalpy of sublimation 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                |

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