

5-Fluorouracil

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| Other names: | 2,4(1H,3H)-Pyrimidinedione, 5-fluoro- 2,4-Pyrimidinedione, 5-fluoro- 5-FU 5-Fluor-2,4-dihydroxypyrimidin 5-Fluor-2,4-pyrimidindiol 5-Fluoracil 5-Fluoro-2,4(1H,3H)-Pyrimidinedione 5-Fluoro-2,4-pyrimidinedione 5-Fluoropyrimidine-2,4-diol 5-Fluoropyrimidine-2,4-dione 5-Fluoruracil 5-Ftouracyl Adrucil Arumel Carac Carzonal Efluderm Efluderm (free base) Efudex Efudix Efurix FU Fluoroblastin Fluoroplex Fluorouracil Fluracil Fluracilum Fluri Fluril Ftoruracil Kecimeton NSC 19893 Queroplex Ro 2-9757 Timazin U-8953 Ulup Uracil, 5-fluoro- |
| Inchi: | InChI=1S/C4H3FN2O2/c5-2-1-6-4(9)7-3(2)8/h1H,(H2,6,7,8,9) |
| InchiKey: | GHASVSINZRGABV-UHFFFAOYSA-N |

Formula: C4H3FN2O2
SMILES: O=c1[nH]cc(F)c(=O)[nH]1
Mol. weight [g/mol]: 130.08
CAS: 51-21-8

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------------|--------|--|
| hsub | 133.20 ± 2.10 | kJ/mol | NIST Webbook |
| log10ws | -1.08 | | Estimated Solubility Method |
| log10ws | -1.03 | | Aqueous and cosolvent solubility data for drug-like organic compounds |
| log10ws | -1.02 | | Aqueous Solubility Prediction Method |
| logp | -1.762 | | Crippen Method |
| mvol | 76.930 | ml/mol | McGowan Method |
| tf | 555.40 | K | Aqueous Solubility Prediction Method |
| tf | 557.15 | K | Solubility of Anti-Inflammatory, Anti-Cancer, and Anti-HIV Drugs in Supercritical Carbon Dioxide |
| tt | 555.66 | K | Measurement and Correlation of the Solubility of 5-Fluorouracil in Pure and Binary Solvents |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|--|
| cps | 143.60 | J/mol×K | 323.15 | Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry |

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|-----|--------|---------|--------|--|
| cps | 142.00 | J/molxK | 318.15 | Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry |
| cps | 153.80 | J/molxK | 343.15 | Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry |
| cps | 150.60 | J/molxK | 338.15 | Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry |
| cps | 147.90 | J/molxK | 333.15 | Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry |
| cps | 145.50 | J/molxK | 328.15 | Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry |
| cps | 140.90 | J/molxK | 313.15 | Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry |
| cps | 140.00 | J/molxK | 308.15 | Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry |

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|-------|---------------|---------|--------|--|
| cps | 139.10 | J/molxK | 303.15 | Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry |
| cps | 138.30 | J/molxK | 298.15 | Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry |
| hsubt | 129.90 | kJ/mol | 397.50 | NIST Webbook |
| hsubt | 150.00 ± 2.00 | kJ/mol | 452.00 | NIST Webbook |
| psub | 1.65e-04 | kPa | 411.14 | Enthalpy of formation of 5-fluoro-1,3-dimethyluracil: 5-Fluorouracil revisited |
| psub | 2.07e-04 | kPa | 413.10 | Enthalpy of formation of 5-fluoro-1,3-dimethyluracil: 5-Fluorouracil revisited |
| psub | 2.39e-04 | kPa | 415.14 | Enthalpy of formation of 5-fluoro-1,3-dimethyluracil: 5-Fluorouracil revisited |
| psub | 2.61e-04 | kPa | 417.14 | Enthalpy of formation of 5-fluoro-1,3-dimethyluracil: 5-Fluorouracil revisited |
| psub | 3.47e-04 | kPa | 419.14 | Enthalpy of formation of 5-fluoro-1,3-dimethyluracil: 5-Fluorouracil revisited |
| psub | 4.18e-04 | kPa | 421.18 | Enthalpy of formation of 5-fluoro-1,3-dimethyluracil: 5-Fluorouracil revisited |
| psub | 4.77e-04 | kPa | 423.16 | Enthalpy of formation of 5-fluoro-1,3-dimethyluracil: 5-Fluorouracil revisited |
| psub | 5.88e-04 | kPa | 425.11 | Enthalpy of formation of 5-fluoro-1,3-dimethyluracil: 5-Fluorouracil revisited |

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| psub | 6.69e-04 | kPa | 427.16 | Enthalpy of formation of 5-fluoro-1,3-dimethyluracil: 5-Fluorouracil revisited |
| psub | 8.36e-04 | kPa | 429.15 | Enthalpy of formation of 5-fluoro-1,3-dimethyluracil: 5-Fluorouracil revisited |
| psub | 1.01e-03 | kPa | 431.11 | Enthalpy of formation of 5-fluoro-1,3-dimethyluracil: 5-Fluorouracil revisited |
| psub | 1.15e-03 | kPa | 433.17 | Enthalpy of formation of 5-fluoro-1,3-dimethyluracil: 5-Fluorouracil revisited |
| psub | 1.66e-04 | kPa | 411.14 | Enthalpy of formation of 5-fluoro-1,3-dimethyluracil: 5-Fluorouracil revisited |
| psub | 1.98e-04 | kPa | 413.10 | Enthalpy of formation of 5-fluoro-1,3-dimethyluracil: 5-Fluorouracil revisited |
| psub | 2.35e-04 | kPa | 415.14 | Enthalpy of formation of 5-fluoro-1,3-dimethyluracil: 5-Fluorouracil revisited |
| psub | 2.83e-04 | kPa | 417.14 | Enthalpy of formation of 5-fluoro-1,3-dimethyluracil: 5-Fluorouracil revisited |
| psub | 3.32e-04 | kPa | 419.14 | Enthalpy of formation of 5-fluoro-1,3-dimethyluracil: 5-Fluorouracil revisited |
| psub | 4.01e-04 | kPa | 421.18 | Enthalpy of formation of 5-fluoro-1,3-dimethyluracil: 5-Fluorouracil revisited |
| psub | 4.72e-04 | kPa | 423.16 | Enthalpy of formation of 5-fluoro-1,3-dimethyluracil: 5-Fluorouracil revisited |
| psub | 5.61e-04 | kPa | 425.11 | Enthalpy of formation of 5-fluoro-1,3-dimethyluracil: 5-Fluorouracil revisited |

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|------|----------|-----|--------|--|
| psub | 6.69e-04 | kPa | 427.16 | Enthalpy of formation of 5-fluoro-1,3-dimethyluracil: 5-Fluorouracil revisited |
| psub | 7.94e-04 | kPa | 429.15 | Enthalpy of formation of 5-fluoro-1,3-dimethyluracil: 5-Fluorouracil revisited |
| psub | 9.61e-04 | kPa | 431.11 | Enthalpy of formation of 5-fluoro-1,3-dimethyluracil: 5-Fluorouracil revisited |
| psub | 1.13e-03 | kPa | 433.17 | Enthalpy of formation of 5-fluoro-1,3-dimethyluracil: 5-Fluorouracil revisited |
| psub | 1.19e-03 | kPa | 433.17 | Enthalpy of formation of 5-fluoro-1,3-dimethyluracil: 5-Fluorouracil revisited |
| psub | 1.03e-03 | kPa | 431.11 | Enthalpy of formation of 5-fluoro-1,3-dimethyluracil: 5-Fluorouracil revisited |
| psub | 8.29e-04 | kPa | 429.15 | Enthalpy of formation of 5-fluoro-1,3-dimethyluracil: 5-Fluorouracil revisited |
| psub | 6.68e-04 | kPa | 427.16 | Enthalpy of formation of 5-fluoro-1,3-dimethyluracil: 5-Fluorouracil revisited |
| psub | 5.80e-04 | kPa | 425.11 | Enthalpy of formation of 5-fluoro-1,3-dimethyluracil: 5-Fluorouracil revisited |
| psub | 4.74e-04 | kPa | 423.16 | Enthalpy of formation of 5-fluoro-1,3-dimethyluracil: 5-Fluorouracil revisited |
| psub | 4.06e-04 | kPa | 421.18 | Enthalpy of formation of 5-fluoro-1,3-dimethyluracil: 5-Fluorouracil revisited |
| psub | 3.51e-04 | kPa | 419.14 | Enthalpy of formation of 5-fluoro-1,3-dimethyluracil: 5-Fluorouracil revisited |

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|------|----------|-----|--------|--|
| psub | 2.78e-04 | kPa | 417.14 | Enthalpy of formation of 5-fluoro-1,3-dimethyluracil: 5-Fluorouracil revisited |
| psub | 2.46e-04 | kPa | 415.14 | Enthalpy of formation of 5-fluoro-1,3-dimethyluracil: 5-Fluorouracil revisited |
| psub | 1.97e-04 | kPa | 413.10 | Enthalpy of formation of 5-fluoro-1,3-dimethyluracil: 5-Fluorouracil revisited |
| psub | 1.78e-04 | kPa | 411.14 | Enthalpy of formation of 5-fluoro-1,3-dimethyluracil: 5-Fluorouracil revisited |

Sources

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| Solubilities in Water of Uracil and Its Halogenated Derivatives: Aqueous and cosolvent solubility data for drug-like organic compounds: Solubility and Chromatographic Separation of 5-Fluorouracil under Subcritical Water Conditions | https://www.doi.org/10.1021/je800029c |
| Solubility and Chromatographic Separation of 5-Fluorouracil under Subcritical Water Conditions | https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/ |
| Solubility and Chromatographic Separation of 5-Fluorouracil under Subcritical Water Conditions | https://www.doi.org/10.1021/acs.jced.7b00015 |
| Solubility and Chromatographic Separation of 5-Fluorouracil under Subcritical Water Conditions | https://www.doi.org/10.1021/je400484u |
| Solubility and Chromatographic Separation of 5-Fluorouracil under Subcritical Water Conditions | http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx |
| Thermodynamic Investigation of Uracil and Its Halo Derivatives. Enthalpies of Sublimation in Methanol: | https://www.doi.org/10.1021/je049656o |
| Thermodynamic Investigation of Uracil and Its Halo Derivatives. Enthalpies of Sublimation in Methanol: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C51218&Units=SI |
| Estimated Solubility Method: | http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt |
| Solubility of Anti-Inflammatory, Anti-Cancer, and Anti-HIV Drugs in Supercritical Carbon Dioxide: | https://www.doi.org/10.1021/je049551l |
| Solubility of Anti-Inflammatory, Anti-Cancer, and Anti-HIV Drugs in Supercritical Carbon Dioxide: | http://link.springer.com/article/10.1007/BF02311772 |
| Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Experimental and Computational Methods | https://www.doi.org/10.1021/je060257y |
| Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Experimental and Computational Methods | https://www.doi.org/10.1016/j.jct.2011.10.020 |
| Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Experimental and Computational Methods | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Measurement and Correlation of the Solubility of 5-Fluorouracil in Pure and Binary Solvents | https://www.doi.org/10.1021/acs.jced.8b00425 |
| Measurement and Correlation of the Solubility of 5-Fluorouracil in Pure and Binary Solvents | https://www.doi.org/10.1016/j.jct.2014.02.018 |

Legend

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| cps: | Solid phase heat capacity |
| hsub: | Enthalpy of sublimation at standard conditions |
| hsubt: | Enthalpy of sublimation at a given temperature |

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| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| psub: | Sublimation pressure |
| tf: | Normal melting (fusion) point |
| tt: | Triple Point Temperature |

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