2,4-Pyrimidinedione, 5-fluoro-

Other names: 2,4(1H,3H)-Pyrimidinedione, 5-fluoro-
5-FU
5-Fluor-2,4-dihydroxypyrimidin
5-Fluor-2,4-pyrimidindiol
5-Fluoracil
5-Fluoro-2,4-pyrimidinedione
5-Fluoropyrimidine-2,4-diol
5-Fluoropyrimidine-2,4-dione
5-Fluoruracil
5-Ftouracyl
5-fluoro-2,4(1H,3H)-pyrimidinedione
5-fluorouracil
Adrucil
Arumel
Carac
Carzonal
Effluderm
Effluderm (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

Physical Properties

Property code	Value	Unit	Source
hf	-450.93	kJ/mol	Cheméo Relay (1.0)
hsub	133.20 ± 2.10	kJ/mol	NIST Webbook
hvap	93.75	kJ/mol	Cheméo Relay (1.0)
ie	9.51	eV	Cheméo Relay (1.0)
log10ws	-1.02		Aqueous Solubility Prediction Method
log10ws	-1.08		Estimated Solubility Method
log10ws	-1.03		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	-1.762		Crippen Method
mcvol	76.930	ml/mol	McGowan Method
tf	557.15	K	Solubility of Anti-Inflammatory, Anti-Cancer, and Anti-HIV Drugs in Supercritical Carbon Dioxide
tf	555.40	K	Aqueous Solubility Prediction Method
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	138.30	J/mol×K	298.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry

cps	153.80	J/mol×K	343.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	150.60	J/mol×K	338.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	147.90	J/mol×K	333.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	145.50	J/mol×K	328.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	143.60	J/mol×K	323.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	142.00	J/mol×K	318.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	140.90	J/mol×K	313.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry

cps	140.00	J/mol×K	308.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	139.10	J/mol×K	303.15	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	1.66e-04	kPa	411.14	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	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

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	1.65e-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	2.07e-04	kPa	413.10	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

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	1.78e-04	kPa	411.14	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
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

Sources

Solubility of Anti-Inflammatory, Anti-Cancer, and Anti-HIV Drugs in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je049551l
Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry:	https://www.doi.org/10.1021/je060257y
Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
Cheméo Relay (1.0):	
Measurement and Correlation of the Solubility of 5-Fluorouracil in Pure and Binary Solvents:	https://www.doi.org/10.1021/acs.jced.8b00425
Enthalpy of formation of 5-fluoro-1,3-dimethyluracil: 5-Fluorouracil revisited:	https://www.doi.org/10.1016/j.jct.2014.02.018
Solubilities in Water of Uracil and Its Halogenated Derivatives:	https://www.doi.org/10.1021/je800029c
Experimental thermochemical study of fluoro-, chloro- and bromo- derivatives of uracil:	https://www.doi.org/10.1016/j.jct.2011.10.020
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51218&Units=SI
Solubility and Chromatographic Separation of 5-Fluorouracil under Subcritical Water Conditions:	https://www.doi.org/10.1021/acs.jced.7b00015
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Cheméo Relay (1.0, beta):	
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubility and Partition Coefficients of 5-Fluorouracil in ScCO2 and ScCO2/Poly(lactic acid):	https://www.doi.org/10.1021/je400484u
Thermodynamic Investigation of Uracil and Its Halo Derivatives. Enthalpies of Solution and Solvation in Methanol:	https://www.doi.org/10.1021/je0496560

Legend

cps: Solid phase heat capacity

hf:	Enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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