2,4(1H,3H)-Pyrimidinedione, 5-(trifluoromethyl)-

Other names:	1,2,3,4-Tetrahydropyrazin-2,4-dione, 5-trifluoromethyl-					
	5-(Trifluoromethyl)uracil					
	5-Trifluoromethyl-1H-pyrimidine-2,4-dione					
	F3T					
	L 595725-0-1					
	TFT					
	Trifluorothymine					
	Uracil, 5-(trifluoromethyl)-					
Inchi:	InChI=1S/C5H3F3N2O2/c6-5(7,8)2-1-9-4(12)10-3(2)11/h1H,(H2,9,10,11,12)					
InchiKey:	LMNPKIOZMGYQIU-UHFFFAOYSA-N					
Formula:	C5H3F3N2O2					
SMILES:	O=c1[nH]cc(C(F)(F)F)c(=O)[nH]1					
Mol. weight [g/mol]:	180.08					
CAS:	54-20-6					

Physical Properties

Property code	Value	Unit	Source
hsub	110.80 ± 0.90	kJ/mol	NIST Webbook
log10ws	0.14		Crippen Method
logp	-0.882		Crippen Method
mcvol	94.560	ml/mol	McGowan Method

Temperature Dependent Properties

cps 192.20 J/mol×K 318.15 Heat Capacities of Uracil, Thymine, and Its Alkylated,	Property code	Value	Unit	Temperature [K]	Source
Cyclooligomethylenate and Halogenated Derivatives by Differential Calorimetry	cps	192.20	J/mol×K	318.15 - Cycl 2	Heat Capacities of Uracil, Thymine, and Its Alkylated, ooligomethylenated, and Halogenated Derivatives by Differential Calorimetry

cps	206.60	J/mol×K	343.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	204.40	J/mol×K	338.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	199.40	J/mol×K	333.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	198.20	J/mol×K	328.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	195.90	J/mol×K	323.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	190.30	J/mol×K	313.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	188.10	J/mol×K	308.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry

cps	183.90	J/mol×K	303.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	182.20	J/mol×K	298.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
hsubt	108.50 ± 0.90	kJ/mol	382.50	NIST Webbook
psub	6.45e-05	kPa	392.01	Vapor pressures, molar enthalpies of sublimation and molar enthalpies of solution in water of 5-trifluoromethyluracil
psub	6.40e-05	kPa	392.01	Vapor pressures, molar enthalpies of sublimation and molar enthalpies of solution in water of 5-trifluoromethyluracil
psub	5.59e-05	kPa	390.15	Vapor pressures, molar enthalpies of sublimation and molar enthalpies of solution in water of 5-trifluoromethyluracil
psub	4.61e-05	kPa	388.25	Vapor pressures, molar enthalpies of sublimation and molar enthalpies of solution in water of 5-trifluoromethyluracil
psub	3.98e-05	kPa	386.35	Vapor pressures, molar enthalpies of sublimation and molar enthalpies of solution in water of 5-trifluoromethyluracil

psub	3.35e-05	kPa	384.45	Vapor pressures, molar enthalpies of sublimation and molar enthalpies of solution in water of 5-trifluoromethyluracil
psub	2.88e-05	kPa	382.54	Vapor pressures, molar enthalpies of sublimation and molar enthalpies of solution in water of 5-trifluoromethyluracil
psub	2.42e-05	kPa	380.67	Vapor pressures, molar enthalpies of sublimation and molar enthalpies of solution in water of 5-trifluoromethyluracil
psub	2.01e-05	kPa	378.75	Vapor pressures, molar enthalpies of sublimation and molar enthalpies of solution in water of 5-trifluoromethyluracil
psub	1.38e-05	kPa	374.94	Vapor pressures, molar enthalpies of sublimation and molar enthalpies of solution in water of 5-trifluoromethyluracil
psub	1.17e-05	kPa	373.02	Vapor pressures, molar enthalpies of sublimation and molar enthalpies of solution in water of 5-trifluoromethyluracil
psub	1.19e-05	kPa	373.02	Vapor pressures, molar enthalpies of sublimation and molar enthalpies of solution in water of 5-trifluoromethyluracil

Sources

Crippen Method:

Crippen Method:

NIST Webbook:

http://pubs.acs.org/doi/abs/10.1021/ci990307I https://www.chemeo.com/doc/models/crippen_log10ws Vapor pressures, molar enthalpies of sublimation and molar enthalp https://www.doi.org/10.1021/je030231w http://link.springer.com/article/10.1007/BF02311772 http://webbook.nist.gov/cgi/cbook.cgi?ID=C54206&Units=SI

Legend

cps:	Solid phase heat capacity
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
psub:	Sublimation pressure

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