

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

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| 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

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|--|
| cps | 192.20 | J/molxK | 318.15 | Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry |

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

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|-------|---------------|---------|--------|--|
| 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 |

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|------|----------|-----|--------|---|
| 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

Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by the Generalized Correspondence Method:
McGowan Method:

<https://www.doi.org/10.1021/je060257y>

<https://www.doi.org/10.1021/je800029c>

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C54206&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Vapor pressures, molar enthalpies of sublimation and molar enthalpies of formation were investigated of Uracil and its Halogen Derivatives. Enthalpies of Solution and Solvation in Methanol:

<https://www.doi.org/10.1021/je030231w>

<https://www.doi.org/10.1021/je049656o>

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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