Theophylline

Other names:

1,3-Dimethylxanthine (theophylline)
1,3-dimethylxanthine
1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-
1H-Purine-2,6-dione, 3,9-dihydro-1,3-dimethyl-
3,7-dihydro-1,3-dimethyl-1H-purine-2,6-dione
Accurbron
Acet-theocin
Aerobin
Aerolate III
Diffumal
Diphyllin
Doraphyllin
Duraphyl
Elixex
Elixicon
Elixophyllin
Elixophylline
Euphylline
GS 2591A
Lanophyllin
Liquophylline
Maphylline
Medaphyllin
NSC 2066
Nuelin
Optiphyllin
Parkophyllin
Physpa
Pseudotheophylline
PulmiDur
Purine-2,6(1H,3H)-dione, 1,3-dimethyl-
Quibron T/SR
Respbid
Slo-Bid
Slo-phyllin
Solosin
Synophylate-L.A. Cenules
Tefamin
Telbans
Teocen 200

Teofilina
Teofyllamin
Teolair
Teonova
Theacitin
Theal tabl.
Theo-11
Theo-Dur
Theocin
Theocontin
Theodel
Theofol
Theograd
Theolair
Theolix
Theona P
Theopek
Theophyl-225
Theophyline
Theophyllin
Theophylline, anhydrous
Theovent
Unicontin CR
Unifyl
Uniphyl
Uniphyllin
X 115
Xanthine, 1,3-dimethyl-
Xanthium
Xantivent

Inchi: InChI=1S/C7H8N4O2/c1-10-5-4(8-3-9-5)6(12)11(2)7(10)13/h3H,1-2H3,(H,8,9)
InchiKey: ZFXYFBGIUFBOJW-UHFFFAOYSA-N
Formula: C7H8N4O2
SMILES: Cn1c(=O)c2[nH]cnc2n(C)c1=O
Mol. weight [g/mol]: 180.16
CAS: 58-55-9

Physical Properties

Property code	Value	Unit	Source

hsub	135.00	kJ/mol	NIST Webbook
log10ws	-3.68		Crippen Method
logp	-1.522		Crippen Method
mcvol	122.230	ml/mol	McGowan Method
rinpol	1900.00		NIST Webbook
rinpol	1990.00		NIST Webbook
rinpol	1900.00		NIST Webbook
rinpol	1917.00		NIST Webbook
rinpol	1917.00		NIST Webbook
rinpol	1917.00		NIST Webbook
rinpol	1947.00		NIST Webbook
rinpol	1921.00		NIST Webbook
rinpol	1917.00		NIST Webbook
rinpol	1917.00		NIST Webbook
rinpol	1962.00		NIST Webbook
rinpol	1923.00		NIST Webbook
rinpol	1904.00		NIST Webbook
rinpol	1909.00		NIST Webbook
tf	544.70 ± 0.50	K	NIST Webbook
tf	545.18	K	Measurement and Correlation of Solubility of Theobromine, Theophylline, and Caffeine in Water and Organic Solvents at Various Temperatures
tf	544.50	K	The physicochemical properties and solubility of pharmaceuticals - Methyl xanthines

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	31.20	kJ/mol	543.70	NIST Webbook
hfust	28.20	kJ/mol	542.30	NIST Webbook
hfust	28.20	kJ/mol	544.00	NIST Webbook
hfust	19.00	kJ/mol	546.80	NIST Webbook
hsubt	126.00	kJ/mol	421.00	NIST Webbook
psub	0.14	kPa	498.00	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds

psub	0.01	kPa	460.40	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds	
psub	0.01	kPa	466.70	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds	
psub	0.02	kPa	468.90	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds	
psub	0.02	kPa	469.80	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds	
psub	0.03	kPa	476.50	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds	
psub	0.04	kPa	478.70	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds	
psub	0.04	kPa	479.20	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds	

psub	0.05	kPa	486.20	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds	
psub	0.07	kPa	488.60	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds	
psub	0.08	kPa	488.60	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds	
psub	0.11	kPa	496.00	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds	
psub	0.01	kPa	459.00	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds	
psub	0.15	kPa	498.50	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds	
psub	0.19	kPa	505.70	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds	

psub	0.23	kPa	507.40	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	0.28	kPa	508.30	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	0.36	kPa	515.50	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	0.39	kPa	516.80	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	0.49	kPa	518.20	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	0.56	kPa	525.20	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	0.82	kPa	526.20	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds

psub	0.90	kPa	528.10	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	1.00	kPa	535.00	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	1.62	kPa	537.90	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	7.20e-03	kPa	457.00	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	6.10e-03	kPa	451.00	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	4.70e-03	kPa	449.10	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	3.30e-03	kPa	447.20	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds

psub	2.80e-03	kPa	441.60	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds

Sources

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

Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds: https://www.doi.org/10.1016/j.tca.2019.05.008

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Volumetric, Viscometric, and 1H NMR Studies on Caffeine, Theophylline, and Theobromine in Aqueous Solutions of $MgCl_2$ at Temperatures T = (288.15 to 318.15) K and at Pressure p = 101.33 kPa: https://www.doi.org/10.1021/acs.jced.7b00520

Volumetric, Viscometric and Spectroscopic Approach to Study the Solvation Behavior of Xanthine Drugs in Aqueous Solutions of $NaSI$ at T = 288.15-318.15 K and at p = 101.325 kPa: https://www.doi.org/10.1021/acs.jced.6b00273

The physicochemical properties and solubility of pharmaceuticals - Methyl xanthines: https://www.doi.org/10.1016/j.jct.2014.05.005

Solubility and Data Correlation of Isoniazid in Different Pure and Binary Mixed Solvent Systems from 283.15 K to 323.15 K: https://www.doi.org/10.1021/acs.jced.8b00785

Solubility of 1,3-Dimethyl-7H-purine-2,6-dione (Theophylline) in Supercritical Carbon Dioxide: https://www.doi.org/10.1021/je900099m

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C58559&Units=SI

Equilibrium partitioning of drug molecules between aqueous and amino acid-ester-based ionic liquids: https://www.doi.org/10.1016/j.jct.2013.02.011

Measurement and Correlation of Solubility of Theobromine, Theophylline, and Caffeine in Water and Organic Solvents at Various Temperatures: https://www.doi.org/10.1021/acs.jced.7b00065

Solid-Liquid Equilibrium of Theophylline in Solvent Mixtures: https://www.doi.org/10.1021/je400864f

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

hfust: Enthalpy of fusion at a given temperature
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
rinpol: Non-polar retention indices
tf: Normal melting (fusion) point

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.