caffeine

Other names:	1,3,7-trimethyl-2,6-dioxopurine
	1,3,7-trimethylxanthine
	1H-purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl-
	3,7-DIHDRO-1,3,7-TRIMETHYL-1H-PURINE-2,6-DIONE
	3,7-dihydro-1,3,7-trimethyl-1H-purine-2,6-dione
	GUARANINE
	METHYLTHEOBROMINE
Inchi:	InChI=1S/C8H10N4O2/c1-10-4-9-6-5(10)7(13)12(3)8(14)11(6)2/h4H,1-3H3
InchiKey:	RYYVLZVUVIJVGH-UHFFFAOYSA-N
Formula:	C8H10N4O2
SMILES:	Cn1c(=O)c2c(ncn2C)n(C)c1=O
Mol. weight [g/mol]:	194.19
CAS:	58-08-2

Physical Properties

Property code	Value	Unit	Source
hfus	3.43	kJ/mol	The standard molar enthalpy of formation, molar heat capacities, and thermal stability of anhydrous caffeine
ie	7.95	eV	NIST Webbook
ie	8.50	eV	NIST Webbook
log10ws	-1.03		Aqueous Solubility Prediction Method
log10ws	-0.88		Estimated Solubility Method
log10ws	-0.95		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	-1.029		Crippen Method
mcvol	136.320	ml/mol	McGowan Method
rinpol	1800.00		NIST Webbook
rinpol	1797.00		NIST Webbook
rinpol	1803.00		NIST Webbook
rinpol	1809.00		NIST Webbook
rinpol	1824.00		NIST Webbook
rinpol	1832.00		NIST Webbook
rinpol	1840.00		NIST Webbook

rinpol	1818.00	NIST Webbook
rinpol	1800.00	NIST Webbook
rinpol	1840.00	NIST Webbook
rinpol	1805.00	NIST Webbook
rinpol	1810.00	NIST Webbook
rinpol	1796.00	NIST Webbook
rinpol	1833.00	NIST Webbook
rinpol	1820.00	NIST Webbook
rinpol	1796.00	NIST Webbook
rinpol	1780.00	NIST Webbook
rinpol	1800.00	NIST Webbook
rinpol	1802.00	NIST Webbook
rinpol	1830.00	NIST Webbook
rinpol	1800.00	NIST Webbook
rinpol	1800.00	NIST Webbook
rinpol	1810.00	NIST Webbook
rinpol	1760.00	NIST Webbook
rinpol	1811.00	NIST Webbook
rinpol	1769.00	NIST Webbook
rinpol	1830.00	NIST Webbook
rinpol	1835.00	NIST Webbook
rinpol	1796.00	NIST Webbook
rinpol	1800.00	NIST Webbook
rinpol	1805.00	NIST Webbook
rinpol	1810.00	NIST Webbook
rinpol	1810.00	NIST Webbook
rinpol	1810.00	NIST Webbook
rinpol	1810.00	NIST Webbook
rinpol	1813.00	NIST Webbook
rinpol	1813.00	NIST Webbook
rinpol	1815.00	NIST Webbook
rinpol	1815.00	NIST Webbook
rinpol	1807.00	NIST Webbook
rinpol	1810.00	NIST Webbook
rinpol	1810.00	NIST Webbook
rinpol	1813.00	NIST Webbook
rinpol	1813.00	NIST Webbook
rinpol	1815.00	NIST Webbook
rinpol	1815.00	NIST Webbook
rinpol	1818.00	NIST Webbook
rinpol	1830.00	NIST Webbook
rinpol	1798.00	NIST Webbook
rinpol	1800.00	NIST Webbook
rinpol	1800.00	NIST Webbook

rinpol	1800.00	NIST Webbook
rinpol	1800.00	NIST Webbook
rinpol	1800.00	NIST Webbook
rinpol	1802.00	NIST Webbook
rinpol	1805.00	NIST Webbook
rinpol	1805.00	NIST Webbook
rinpol	1805.00	NIST Webbook
rinpol	1810.00	NIST Webbook
rinpol	1850.00	NIST Webbook
rinpol	1768.00	NIST Webbook
rinpol	1764.00	NIST Webbook
rinpol	1840.00	NIST Webbook
rinpol	1768.00	NIST Webbook
rinpol	1775.00	NIST Webbook
rinpol	1778.00	NIST Webbook
rinpol	1761.00	NIST Webbook
rinpol	1800.00	NIST Webbook
rinpol	1768.00	NIST Webbook
rinpol	1838.00	NIST Webbook
rinpol	1809.00	NIST Webbook
rinpol	1775.00	NIST Webbook
rinpol	1789.00	NIST Webbook
rinpol	1800.00	NIST Webbook
rinpol	1806.00	NIST Webbook
rinpol	1810.00	NIST Webbook
rinpol	1810.00	NIST Webbook
rinpol	1810.00	NIST Webbook
rinpol	1789.00	NIST Webbook
rinpol	1772.00	NIST Webbook
rinpol	1836.00	NIST Webbook
rinpol	1842.00	NIST Webbook
rinpol	1800.00	NIST Webbook
rinpol	1774.00	NIST Webbook
rinpol	1779.00	NIST Webbook
rinpol	1784.00	NIST Webbook
rinpol	1800.00	NIST Webbook
rinpol	1776.00	NIST Webbook
rinpol	1775.00	NIST Webbook
rinpol	1768.00	NIST Webbook
rinpol	1764.00	NIST Webbook
rinpol	1815.00	NIST Webbook
rinpol	1797.00	NIST Webbook
rinpol	1797.00	NIST Webbook
rinpol	1790.00	NIST Webbook

rinpol	1790.00		NIST Webbook
rinpol	1841.00		NIST Webbook
rinpol	1837.00		NIST Webbook
rinpol	1805.00		NIST Webbook
rinpol	1771.00		NIST Webbook
rinpol	1820.00		NIST Webbook
rinpol	1810.00		NIST Webbook
rinpol	1775.00		NIST Webbook
rinpol	1810.00		NIST Webbook
rinpol	1776.00		NIST Webbook
rinpol	1777.00		NIST Webbook
rinpol	1810.00		NIST Webbook
rinpol	1801.00		NIST Webbook
rinpol	1810.00		NIST Webbook
rinpol	306.60		NIST Webbook
rinpol	1820.00		NIST Webbook
rinpol	1760.00		NIST Webbook
rinpol	1796.00		NIST Webbook
rinpol	1810.00		NIST Webbook
rinpol	1815.00		NIST Webbook
rinpol	1813.00		NIST Webbook
rinpol	1798.00		NIST Webbook
rinpol	1800.00		NIST Webbook
rinpol	1768.00		NIST Webbook
rinpol	1830.00		NIST Webbook
rinpol	1841.00		NIST Webbook
rinpol	1848.00		NIST Webbook
rinpol	1832.00		NIST Webbook
rinpol	1760.00		NIST Webbook
tf	510.40	K	Aqueous Solubility Prediction Method
tf	510.15	K	Thermodynamic modeling studies of aqueous solubility of caffeine, gallic acid and their cocrystal in the temperature range of 303 K-363 K
tf	505.40	K	Solubility of high-value compounds in ethyl lactate: Measurements and modelling
tf	508.75	K	DSC study and phase diagrams calculation of binary systems of paracetamol
tf	509.35	K	Artificial neural networks as a supporting tool for compatibility study based on thermogravimetric data

tf	509.07	K	Measurement and Correlation of Solubility of Theobromine, Theophylline, and Caffeine in Water and Organic Solvents at Various Temperatures
tf	509.30 ± 0.10	K	NIST Webbook
tf	508.00 ± 1.00	K	NIST Webbook
tt	508.30 ± 1.50	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	232.00	J/mol×K	298.15	NIST Webbook
cps	173.20	J/mol×K	298.00	NIST Webbook
hfust	19.86	kJ/mol	509.50	NIST Webbook
hfust	20.95	kJ/mol	508.30	NIST Webbook
hfust	21.90	kJ/mol	510.20	NIST Webbook
hfust	24.80	kJ/mol	507.70	NIST Webbook
hfust	18.30	kJ/mol	510.00	NIST Webbook
hfust	19.38	kJ/mol	510.20	NIST Webbook
hsubt	112.60 ± 2.40	kJ/mol	339.50	NIST Webbook
hsubt	103.60	kJ/mol	423.00	NIST Webbook
hvapt	64.90 ± 2.40	kJ/mol	688.50	NIST Webbook
psub	0.07	kPa	437.40	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	6.93e-03	kPa	410.10	Thermodynamic properties of caffeine: Reconciliation of available experimental data
psub	3.10e-03	kPa	394.70	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds

psub	3.50e-03	kPa	398.40	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	3.90e-03	kPa	399.80	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	6.70e-03	kPa	404.10	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	9.20e-03	kPa	408.20	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	9.90e-03	kPa	409.70	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	0.01	kPa	413.50	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	0.02	kPa	417.90	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds

psub	0.02	kPa	419.50	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	0.02	kPa	422.80	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	0.03	kPa	427.70	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	0.04	kPa	429.40	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	0.05	kPa	432.20	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	5.77e-03	kPa	408.00	Thermodynamic properties of caffeine: Reconciliation of available experimental data
psub	0.07	kPa	439.30	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	0.09	kPa	441.60	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds

psub	0.13	kPa	447.20	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds	
psub	0.16	kPa	449.10	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds	
psub	0.16	kPa	451.00	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds	
psub	0.23	kPa	457.00	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds	
psub	0.26	kPa	459.00	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds	
psub	0.29	kPa	460.40	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds	
psub	0.41	kPa	466.70	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds	

psub	0.48	kPa	468.90	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	0.49	kPa	469.80	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	0.72	kPa	476.50	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	0.83	kPa	478.70	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	0.91	kPa	479.20	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	1.08	kPa	486.20	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	1.42	kPa	488.60	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	5.25e-03	kPa	406.00	Thermodynamic properties of caffeine: Reconciliation of available experimental data

psub	4.41e-03	kPa	405.00	Thermodynamic properties of caffeine: Reconciliation of available experimental data
psub	3.38e-03	kPa	400.90	Thermodynamic properties of caffeine: Reconciliation of available experimental data
psub	2.23e-03	kPa	395.90	Thermodynamic properties of caffeine: Reconciliation of available experimental data
psub	1.06e-03	kPa	386.90	Thermodynamic properties of caffeine: Reconciliation of available experimental data
psub	7.70e-04	kPa	383.90	Thermodynamic properties of caffeine: Reconciliation of available experimental data
psub	5.50e-04	kPa	379.90	Thermodynamic properties of caffeine: Reconciliation of available experimental data
psub	3.30e-04	kPa	373.30	Thermodynamic properties of caffeine: Reconciliation of available experimental data
psub	1.70e-04	kPa	366.20	Thermodynamic properties of caffeine: Reconciliation of available experimental data
psub	1.28e-03	kPa	389.80	Thermodynamic properties of caffeine: Reconciliation of available experimental data

Sources

Solubility of Azoxystrobin and Benflumetol in Compressed CO2 Measured by the Static Precise Mass Measuring Method:	https://www.doi.org/10.1021/acs.jced.8b00388
Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
DSC study and phase diagrams calculation of binary systems of paracetamol:	https://www.doi.org/10.1016/j.tca.2012.09.024
Thermodynamic modeling studies of aqueous solubility of caffeine, gallic acid and their cocrystal in the temperature range of 303 K-363 K:	https://www.doi.org/10.1016/j.fluid.2017.09.021
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C58082&Units=SI
Solubility of high-value compounds in environmentally friendly solvents liquid poly(ethylene glycol) and ionic liquids:	https://www.doi.org/10.1016/j.jct.2013.10.036
Measurement and Correlation of Solubility of Theobromine, Theophylline, and Caffeine in Various Solvents at Various Temperatures:	https://www.doi.org/10.1021/acs.jced.7b00065
Solubility Study and Thermodynamic Analysis of Caffeine in Water and Organic Solvents at Various Temperatures:	https://www.doi.org/10.1021/acs.jced.7b00520
Volumetric, Viscometric, and 1H NMR Studies on Caffeine, Theophylline, and Theobromine in Aqueous Solutions of MgCl2 at Temperatures T = (288.15 to 318.15) K and at Pressure p = 101.3 kPa:	http://link.springer.com/article/10.1007/BF02311772
The standard molar enthalpy of formation, molar heat capacities, and thermal stability of anhydrous caffeine:	https://www.doi.org/10.1016/j.jct.2006.05.009
Solubility of high-value compounds in ethyl lactate: Measurements and modeling:	https://www.doi.org/10.1016/j.jct.2011.12.005
Thermodynamic properties of caffeine: Reconciliation of available experimental data:	https://www.doi.org/10.1016/j.jct.2008.07.002
Apparent molar volumes and viscosity B-coefficients of caffeine in aqueous thorium nitrate solutions at T = (298.15, 308.15, and 318.15) K:	https://www.doi.org/10.1016/j.jct.2009.09.010
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1479
Volumetric, Viscometric and Spectroscopic Approach to Study the Solvation Behavior of Xanthine Drugs in Aqueous Solutions of NaCl at T = (293.15, 298.15, 303.15, and 308.15) K and at P = 100.85 kPa:	https://www.doi.org/10.1021/acs.jced.6b00273
Artificial neural networks as a supporting tool for compatibility study between pharmaceutical drugs and excipients:	https://www.doi.org/10.1016/j.tca.2017.12.015
Solubility and partitioning of drug molecules between aqueous and amino acid–caffeine ionic liquids:	https://www.doi.org/10.1016/j.jct.2013.02.011
Effect of caffeine on the Physicochemical Properties of Neurotransmitter GABA:	https://www.doi.org/10.1021/acs.jced.9b00327
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Thermodynamic and Theoretical Approach:	https://www.doi.org/10.1016/j.tca.2019.05.008
Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds:	

Legend

cps:	Solid phase heat capacity
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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
tt:	Triple Point Temperature