Benzoic acid, 4-methyl-

Other names:	4-Methylbenzoic acid
	4-Toluic acid
	Crithminic acid
	NSC 2215
	p-Carboxytoluene
	p-Methylbenzoic acid
	p-Toluic acid
	p-Toluylic acid
	p-Tolylcarboxylic acid
	para-Toluic acid
Inchi:	InChI=1S/C8H8O2/c1-6-2-4-7(5-3-6)8(9)10/h2-5H,1H3,(H,9,10)
InchiKey:	LPNBBFKOUUSUDB-UHFFFAOYSA-N
Formula:	C8H8O2
SMILES:	Cc1ccc(C(=O)O)cc1
Mol. weight [g/mol]:	136.15
CAS:	99-94-5

Physical Properties

Property code	Value	Unit	Source
affp	836.70	kJ/mol	NIST Webbook
basg	805.70	kJ/mol	NIST Webbook
chs	-3862.30 ± 0.90	kJ/mol	NIST Webbook
chs	-3862.30 ± 0.92	kJ/mol	NIST Webbook
chs	-3868.00	kJ/mol	NIST Webbook
gf	-146.48	kJ/mol	Joback Method
hf	-330.40 ± 1.50	kJ/mol	NIST Webbook
hf	-330.40	kJ/mol	NIST Webbook
hf	-324.50	kJ/mol	NIST Webbook
hfs	-423.30 ± 3.80	kJ/mol	NIST Webbook
hfs	-429.20 ± 1.10	kJ/mol	NIST Webbook
hfs	-429.20 ± 1.50	kJ/mol	NIST Webbook
hfus	22.48	kJ/mol	Thermodynamic study of the sublimation of eight 4-n-alkylbenzoic acids
hsub	98.80	kJ/mol	NIST Webbook
hsub	98.80 ± 0.30	kJ/mol	NIST Webbook
hsub	98.80 ± 0.30	kJ/mol	NIST Webbook

hsub	98.60 ± 0.60	kJ/mol	NIST Webbook
hvap	59.77	kJ/mol	Joback Method
ie	9.40	eV	NIST Webbook
ie	9.20 ± 0.20	eV	NIST Webbook
log10ws	-2.60		Aqueous Solubility Prediction Method
logp	1.693		Crippen Method
mcvol	107.260	ml/mol	McGowan Method
pc	4356.87	kPa	Joback Method
rinpol	1213.00		NIST Webbook
rinpol	1213.00		NIST Webbook
rinpol	1213.00		NIST Webbook
tb	547.70	K	NIST Webbook
tc	775.00	K	Vapor-liquid critical point measurements of fifteen compounds by the pulse-heating method
tf	453.46	K	Aqueous Solubility Prediction Method
tf	450.15 ± 2.50	K	NIST Webbook
tf	455.00 ± 2.00	K	NIST Webbook
tf	455.10	K	Solid-Liquid Equilibria for Benzoic Acid + p-Toluic Acid + Chloroform, Benzoic Acid + p-Toluic Acid + Acetic Acid, and Terephthalic Acid + Isophthalic Acid + N,N-Dimethylformamide
tf	453.30	K	Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods
tf	452.80 ± 0.30	K	NIST Webbook
vc	0.401	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.03	J/mol×K	732.94	Joback Method
cpg	235.84	J/mol×K	560.15	Joback Method
cpg	245.16	J/mol×K	594.71	Joback Method
cpg	253.91	J/mol×K	629.27	Joback Method
cpg	262.13	J/mol×K	663.82	Joback Method
cpg	269.83	J/mol×K	698.38	Joback Method

cpg	283.75	J/mol×K	767.50	Joback Method
cps	169.00	J/mol×K	298.00	NIST Webbook
dvisc	0.0001208	Pa×s	560.15	Joback Method
dvisc	0.0051891	Pa×s	329.61	Joback Method
dvisc	0.0019990	Pa×s	368.03	Joback Method
dvisc	0.0009222	Pa×s	406.46	Joback Method
dvisc	0.0004863	Pa×s	444.88	Joback Method
dvisc	0.0002839	Pa×s	483.30	Joback Method
dvisc	0.0001794	Pa×s	521.73	Joback Method
hfust	22.72	kJ/mol	452.80	NIST Webbook
hfust	22.72	kJ/mol	452.80	NIST Webbook
hfust	22.72	kJ/mol	452.80	NIST Webbook
sfust	50.20	J/mol×K	452.80	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54810e+01
Coeff. B	-4.80703e+03
Coeff. C	-1.05173e+02
Temperature range (K), min.	421.56
Temperature range (K), max.	577.86

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.46674e+02
Coeff. B	-1.53125e+04
Coeff. C	-1.83932e+01
Coeff. D	6.20185e-06
Temperature range (K), min.	452.75
Temperature range (K), max.	773.00

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Measurement and Correlation of the Solubility for Camptothecine in Different Organic Solvents: https://www.doi.org/10.1021/acs.jced.5b00994

The effect of temperature on the solubility of benzoic acid derivatives in water: https://www.doi.org/10.1016/j.fluid.2006.10.014

Determination and modeling of aqueous solubility of 4-position substituted benzoic acid compounds in a high-temperature solution: https://www.doi.org/10.1016/j.fluid.2012.11.023

Solubilities of Benzene Carboxylic Acids in Isobutyl Acetate from (299.73 to 355.15) K: https://www.doi.org/10.1021/je101319f

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

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=957

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C99945&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Solid-Liquid Equilibrium Solubility, Thermodynamic Properties, and Molecular Simulation of Phenylphosphonic Acid in 15 Pure Solvents at Different Temperatures: https://www.doi.org/10.1021/acs.jced.9b00362

Vapor–liquid critical point measurements of fifteen compounds by the pulse-heating method: https://www.doi.org/10.1016/j.fluid.2014.07.038

Solid–Liquid Equilibria of Several Systems Containing Acetic Acid: https://www.doi.org/10.1021/je034114c

Solubilities of Benzoic Acid, p-Methylbenzoic Acid, m-Methylbenzoic Acid, o-Methylbenzoic Acid, p-Hydroxybenzoic Acid, and o-Nitrobenzoic Acid in 1-Octanol: https://www.doi.org/10.1021/je700677d

Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods: https://www.doi.org/10.1016/j.tca.2015.03.026

Solid-Liquid Equilibria for Benzoic Acid + p-Toluic Acid + Chloroform, Benzoic Acid + p-Toluic Acid + Acetic Acid, and Terephthalic Acid + Isophthalic Acid + N,N-Dimethylformamide: https://www.doi.org/10.1021/je049801y

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Thermodynamic study of the sublimation of eight 4-n-alkylbenzoic acids: https://www.doi.org/10.1016/j.jct.2004.02.001

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

Solubility and partition coefficient of p-toluic acid in p-xylene and water: https://www.doi.org/10.1016/j.fluid.2012.12.009

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=957

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
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
pc:	Critical Pressure

pvap:	Vapor pressure
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume