Benzoic acid, 2-methyl-

Other names:	2-Methylbenzoic acid
	Orthotoluic acid
	o-Methylbenzoic acid
	o-Toluic acid
	o-Toluylic acid
Inchi:	InChI=1S/C8H8O2/c1-6-4-2-3-5-7(6)8(9)10/h2-5H,1H3,(H,9,10)
InchiKey:	ZWLPBLYKEWSWPD-UHFFFAOYSA-N
Formula:	C8H8O2
SMILES:	Cc1ccccc1C(=O)O
Mol. weight [g/mol]:	136.15
CAS:	118-90-1

Physical Properties

Property code	Value	Unit	Source
affp	838.80	kJ/mol	NIST Webbook
basg	807.80	kJ/mol	NIST Webbook
chs	-3875.00 ± 0.75	kJ/mol	NIST Webbook
chs	-3864.00	kJ/mol	NIST Webbook
chs	-3874.40 ± 4.60	kJ/mol	NIST Webbook
chs	-3858.00	kJ/mol	NIST Webbook
chs	-3874.90 ± 0.80	kJ/mol	NIST Webbook
gf	-146.48	kJ/mol	Joback Method
hf	-331.20	kJ/mol	NIST Webbook
hf	-320.60	kJ/mol	NIST Webbook
hf	-320.60 ± 1.50	kJ/mol	NIST Webbook
hfs	-427.10 ± 3.80	kJ/mol	NIST Webbook
hfs	-416.50 ± 0.92	kJ/mol	NIST Webbook
hfs	-416.50 ± 1.50	kJ/mol	NIST Webbook
hfus	15.81	kJ/mol	Joback Method
hsub	95.90 ± 0.10	kJ/mol	NIST Webbook
hsub	95.90	kJ/mol	NIST Webbook
hsub	95.90 ± 0.10	kJ/mol	NIST Webbook
hvap	59.77	kJ/mol	Joback Method
ie	9.40	eV	NIST Webbook
ie	9.10	eV	NIST Webbook
log10ws	-2.06		Aqueous Solubility Prediction Method

logp	1.693		Crippen Method
mcvol	107.260	ml/mol	McGowan Method
pc	4356.87	kPa	Joback Method
tb	531.70	K	NIST Webbook
tc	763.00	K	Vapor-liquid critical point measurements of fifteen compounds by the pulse-heating method
tf	376.50 ± 0.05	K	NIST Webbook
tf	377.65 ± 2.00	K	NIST Webbook
tf	376.90 ± 0.30	K	NIST Webbook
tf	377.63	K	Aqueous Solubility Prediction Method
tf	380.00 ± 1.50	K	NIST Webbook
vc	0.401	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.13	J/mol×K	663.82	Joback Method
cpg	245.16	J/mol×K	594.71	Joback Method
cpg	235.84	J/mol×K	560.15	Joback Method
cpg	269.83	J/mol×K	698.38	Joback Method
cpg	277.03	J/mol×K	732.94	Joback Method
cpg	283.75	J/mol×K	767.50	Joback Method
cpg	253.91	J/mol×K	629.27	Joback Method
cps	174.90	J/mol×K	298.00	NIST Webbook
dvisc	0.0009222	Pa×s	406.46	Joback Method
dvisc	0.0004863	Pa×s	444.88	Joback Method
dvisc	0.0051891	Pa×s	329.61	Joback Method
dvisc	0.0002839	Pa×s	483.30	Joback Method
dvisc	0.0001794	Pa×s	521.73	Joback Method
dvisc	0.0001208	Pa×s	560.15	Joback Method
dvisc	0.0019990	Pa×s	368.03	Joback Method
hfust	20.17	kJ/mol	376.90	NIST Webbook
hfust	20.17	kJ/mol	376.90	NIST Webbook
hfust	20.17	kJ/mol	376.90	NIST Webbook

psub	2.80e-03	kPa	331.20	Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods
psub	0.13	kPa	373.00	Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods
psub	0.08	kPa	367.40	Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods
psub	0.07	kPa	364.20	Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods
psub	0.05	kPa	361.20	Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods
psub	0.04	kPa	358.70	Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods
psub	0.04	kPa	358.60	Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods

psub	0.03	kPa	355.40	Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods
psub	0.02	kPa	351.20	Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods
psub	0.02	kPa	348.20	Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods
psub	0.01	kPa	345.20	Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods
psub	7.67e-03	kPa	341.20	Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods
psub	4.21e-03	kPa	335.20	Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods
sfust	53.50	J/mol×K	376.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54533e+01
Coeff. B	-4.69014e+03
Coeff. C	-9.91310e+01
Temperature range (K), min.	376.85
Temperature range (K), max.	561.58

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.31614e+02
Coeff. B	-1.40488e+04
Coeff. C	-1.62792e+01
Coeff. D	5.55990e-06
Temperature range (K), min.	376.85
Temperature range (K), max.	751.00

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C118901&Units=SI
Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods:	https://www.doi.org/10.1016/j.tca.2015.03.026
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=956
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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=956
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Vapor-liquid critical point measurements of fifteen compounds by the pulse heating method:	https://www.doi.org/10.1016/j.fluid.2014.07.038
Solubilities of Phthalic Acid and o-Toluic Acid in Binary Acetic Acid + Water and Acetic Acid + o-Xylene Solvent Mixtures:	https://www.doi.org/10.1021/acs.jced.6b00324

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
psub:	Sublimation pressure
pvap:	Vapor pressure
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume