

Benzoic acid, 3-methyl-

Other names:	3-Methylbenzoic acid m-Methylbenzoic acid m-Toluic acid m-Toluyllic acid meta-Toluic acid
Inchi:	InChI=1S/C8H8O2/c1-6-3-2-4-7(5-6)8(9)10/h2-5H,1H3,(H,9,10)
InchiKey:	GPSDUZXPYCFOSQ-UHFFFAOYSA-N
Formula:	C8H8O2
SMILES:	Cc1cccc(C(=O)O)c1
Mol. weight [g/mol]:	136.15
CAS:	99-04-7

Physical Properties

Property code	Value	Unit	Source
affp	829.80	kJ/mol	NIST Webbook
basg	798.80	kJ/mol	NIST Webbook
chs	-3862.00	kJ/mol	NIST Webbook
chs	-3866.50 ± 0.90	kJ/mol	NIST Webbook
chs	-3865.30 ± 0.79	kJ/mol	NIST Webbook
gf	-146.48	kJ/mol	Joback Method
hf	-329.10	kJ/mol	NIST Webbook
hf	-327.90 ± 1.40	kJ/mol	NIST Webbook
hfs	-426.10 ± 0.96	kJ/mol	NIST Webbook
hfs	-424.90 ± 1.40	kJ/mol	NIST Webbook
hfus	15.81	kJ/mol	Joback Method
hsub	97.00	kJ/mol	NIST Webbook
hsub	97.00 ± 0.30	kJ/mol	NIST Webbook
hsub	97.00 ± 0.30	kJ/mol	NIST Webbook
hvap	59.77	kJ/mol	Joback Method
ie	9.40 ± 0.20	eV	NIST Webbook
log10ws	-2.14		Aqueous Solubility Prediction Method
logp	1.693		Crippen Method
mcvol	107.260	ml/mol	McGowan Method
pc	4356.87	kPa	Joback Method
rinpol	1249.00		NIST Webbook
rinpol	1325.00		NIST Webbook

tb	536.20	K	NIST Webbook
tc	771.00	K	Vapor-liquid critical point measurements of fifteen compounds by the pulse-heating method
tf	381.90 ± 0.20	K	NIST Webbook
tf	384.40 ± 2.00	K	NIST Webbook
tf	382.40	K	Abraham model correlations for describing the thermodynamic properties of solute transfer into pentyl acetate based on headspace chromatographic and solubility measurements
tf	383.07	K	Aqueous Solubility Prediction Method
tf	384.00 ± 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	253.91	J/mol×K	629.27	Joback Method
cpg	283.75	J/mol×K	767.50	Joback Method
cpg	277.03	J/mol×K	732.94	Joback Method
cpg	269.83	J/mol×K	698.38	Joback Method
cpg	235.84	J/mol×K	560.15	Joback Method
cpg	245.16	J/mol×K	594.71	Joback Method
cps	163.60	J/mol×K	298.00	NIST Webbook
dvisc	0.0019990	Paxs	368.03	Joback Method
dvisc	0.0009222	Paxs	406.46	Joback Method
dvisc	0.0004863	Paxs	444.88	Joback Method
dvisc	0.0002839	Paxs	483.30	Joback Method
dvisc	0.0001794	Paxs	521.73	Joback Method
dvisc	0.0051891	Paxs	329.61	Joback Method
dvisc	0.0001208	Paxs	560.15	Joback Method
hfust	15.73	kJ/mol	381.90	NIST Webbook
hfust	15.73	kJ/mol	381.90	NIST Webbook
hfust	15.73	kJ/mol	381.90	NIST Webbook
hvapt	62.80	kJ/mol	503.00	NIST Webbook
sfust	41.20	J/mol×K	381.90	NIST Webbook

Sources

Vapor-liquid critical point measurements of fifteen compounds by open Method:	https://www.doi.org/10.1016/j.fluid.2014.07.038 http://pubs.acs.org/doi/abs/10.1021/ci990307l
Abraham model correlations for describing the thermodynamic properties of solute transfer into pentyl Acetate, Benzene, Acetone, Acetone-Acidspace, and Aqueous 1-Octanol. Joback Method: Methylbenzoic Acid, p-Hydroxybenzoic Acid, and <i>p</i> -Nitrobenzoic Acid in 1-Octanol: Joback Method:	https://www.doi.org/10.1016/j.jct.2018.05.003 https://www.doi.org/10.1021/je700677d http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa http://link.springer.com/article/10.1007/BF02311772 https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C99047&Units=SI
The effect of temperature on the solubility of benzoic acid derivatives in water:	https://www.doi.org/10.1016/j.fluid.2006.10.014

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
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
pc:	Critical 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

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