M-TOLUIC ACID

Other names: 3-methylbenzoic acid
benzoic acid, 3-methyl-
m-Methylbenzoic acid
m-Toluylic 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

Physical Properties

Property code	Value	Unit	Source
af	0.6555		Cheméo Relay (1.0)
affp	829.80	kJ/mol	NIST Webbook
basg	798.80	kJ/mol	NIST Webbook
chs	-3866.50 ± 0.90	kJ/mol	NIST Webbook
chs	-3865.30 ± 0.79	kJ/mol	NIST Webbook
chs	-3862.00	kJ/mol	NIST Webbook
gf	-146.48	kJ/mol	Joback Method
hf	-327.90 ± 1.40	kJ/mol	NIST Webbook
hf	-329.10	kJ/mol	NIST Webbook
hfs	-424.90 ± 1.40	kJ/mol	NIST Webbook
hfs	-426.10 ± 0.96	kJ/mol	NIST Webbook
hfus	15.81	kJ/mol	Joback Method
hsub	97.00 ± 0.30	kJ/mol	NIST Webbook
hsub	97.00 ± 0.30	kJ/mol	NIST Webbook
hsub	97.00 ± 0.30	kJ/mol	NIST Webbook
hsub	97.00	kJ/mol	NIST Webbook
hsub	97.00	kJ/mol	NIST Webbook
hsub	97.00 ± 0.30	kJ/mol	NIST Webbook
hvap	84.76	kJ/mol	Cheméo Relay (1.0)
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	381.90 ± 0.20	K	NIST Webbook
tf	384.40 ± 2.00	K	NIST Webbook
tf	384.00 ± 1.50	K	NIST Webbook
tf	383.07	K	Aqueous Solubility Prediction Method
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
vc	0.380	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	277.03	J/mol×K	732.94	Joback Method
cpg	283.75	J/mol×K	767.50	Joback Method
cps	163.60	J/mol×K	298.00	NIST Webbook
dvisc	0.0004863	Pa×s	444.88	Joback Method
dvisc	0.0009222	Pa×s	406.46	Joback Method
dvisc	0.0019990	Pa×s	368.03	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	0.0051891	Pa×s	329.61	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

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
sfust	41.20	J/mol×K	381.90	NIST Webbook

Sources

Cheméo Relay (1.0):

Vapor-liquid critical point measurements of fifteen compounds by the pulse-heating method:	https://www.doi.org/10.1016/j.fluid.2014.07.038
Abraham model correlations for describing the thermodynamic properties of solute transfer into pentyl acetate based on headspace chromatographic and solubility measurements:	https://www.doi.org/10.1016/j.jct.2018.05.003
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
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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Cheméo Relay (1.0, beta):

Legend

af:	Acentric Factor
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