Terephthalic acid

Other names:	1,4-Benzenedicarboxylic acid
	1,4-Dicarboxybenzene
	1,4-benzenedioic acid
	Acide terephtalique
	Benzene, 1,4-dicarboxylic acid
	Benzene, p-dicarboxylic acid
	Kyselina tereftalova
	NSC 36973
	TA 12
	TPA
	Ta-33mp
	WR 16262
	p-Benzenedicarboxylic acid
	p-Carboxybenzoic acid
	p-Dicarboxybenzene
	p-Phthalic acid
Inchi:	InChI=1S/C8H6O4/c9-7(10)5-1-2-6(4-3-5)8(11)12/h1-4H,(H,9,10)(H,11,12)
InchiKey:	KKEYFWRCBNTPAC-UHFFFAOYSA-N
Formula:	C8H6O4
SMILES:	O=C(O)c1ccc(C(=O)O)cc1
Mol. weight [g/mol]:	166.13
CAS:	100-21-0

Physical Properties

Property code	Value	Unit	Source
chs	-3227.96	kJ/mol	NIST Webbook
chs	-3189.30 ± 1.50	kJ/mol	NIST Webbook
chs	-3189.50 ± 0.42	kJ/mol	NIST Webbook
gf	-412.22	kJ/mol	Joback Method
hf	-513.01	kJ/mol	Joback Method
hfs	-816.17	kJ/mol	NIST Webbook
hfs	-816.30 ± 1.50	kJ/mol	NIST Webbook
hfus	21.50	kJ/mol	Joback Method
hsub	98.11	kJ/mol	NIST Webbook
hsub	146.60 ± 0.50	kJ/mol	NIST Webbook
hvap	83.19	kJ/mol	Joback Method
ie	9.90 ± 0.20	eV	NIST Webbook

log10ws	-1.59		Crippen Method
logp	1.083		Crippen Method
mcvol	114.700	ml/mol	McGowan Method
pc	5406.57	kPa	Joback Method
tb	706.20	K	Joback Method
tc	907.67	K	Joback Method
tf	703.10	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
vc	0.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.34	J/mol×K	840.51	Joback Method
cpg	301.12	J/mol×K	806.93	Joback Method
cpg	315.57	J/mol×K	907.67	Joback Method
cpg	311.15	J/mol×K	874.09	Joback Method
cpg	282.80	J/mol×K	706.20	Joback Method
cpg	289.37	J/mol×K	739.78	Joback Method
cpg	295.47	J/mol×K	773.36	Joback Method
cps	199.60	J/mol×K	323.00	NIST Webbook
dvisc	0.0000196	Pa×s	706.20	Joback Method
dvisc	0.0001006	Pa×s	573.28	Joback Method
dvisc	0.0000539	Pa×s	617.59	Joback Method
dvisc	0.0000314	Pa×s	661.89	Joback Method
dvisc	0.0013822	Pa×s	440.36	Joback Method
dvisc	0.0004918	Pa×s	484.67	Joback Method
dvisc	0.0002081	Pa×s	528.97	Joback Method
hsubt	131.00	kJ/mol	578.00	NIST Webbook
hsubt	139.30 ± 3.80	kJ/mol	621.50	NIST Webbook
hsubt	139.20	kJ/mol	578.00	NIST Webbook
hsubt	142.20 ± 1.50	kJ/mol	471.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	4.38606e+02
Coeff. B	-3.45524e+04
Coeff. C	-6.04690e+01
Coeff. D	2.04789e-05
Temperature range (K), min.	567.15
Temperature range (K), max.	1113.00

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubilities of Terephthalic Acid in Dimethyl Sulfoxide + Water and in N,N-Dimethylformamide + Water from (301.15 to 373.2) K:	https://www.doi.org/10.1021/je049577c
Phase Equilibrium and Phase Diagram for the System of Benzene Dicarboxylic Acid + N-Methyl-2-pyrrolidone:	https://www.doi.org/10.1021/je500542j
Solubility of 2,5-Furandicarboxylic Acid in Eight Pure Solvents and Two Binary Solvent Systems at 313.15-363.15 K:	https://www.doi.org/10.1021/acs.jced.7b00927
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Solubility of terephthalic acid in aqueous acetic acid from 423.15 to 513.15K:	https://www.doi.org/10.1016/j.fluid.2005.04.015
Solubilities of 4-Carboxybenzaldehyde and 1,4-Benzenedicarboxylic Acid in N-Methyl-2-pyrrolidone in the Temperature Range from (343.2 to 468.2) K:	https://www.doi.org/10.1021/je049706p
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C100210&Units=SI
Solid-Liquid Equilibria of Several Systems Containing Acetic Acid:	https://www.doi.org/10.1021/je034114c
Solubility of Terephthalic Acid in Aqueous N-Methyl Pyrrolidone and N,N-Dimethyl Acetamide Solvents at (301.2 to 369.2) K:	https://www.doi.org/10.1021/je700635r
Solid-liquid Equilibria for Benzoic Acid + 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
Solubility of Terephthalic Acid in Subcritical Water:	https://www.doi.org/10.1021/je300263z
The solubilities of benzene polycarboxylic acids in water:	https://www.doi.org/10.1016/j.jct.2005.07.007
Solubilities of Benzene Carboxylic Acids in Isobutyl Acetate from (299.73 to 353.15) K:	https://www.doi.org/10.1021/je101319f
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
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=969
Thermochemistry of Cs(hydrogen phthalate) and Cs2(terephthalate):	https://www.doi.org/10.1016/j.tca.2005.01.024
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Solubilities of Terephthalic Acid, Phthalic Acid, and Isophthalic Acid in Tetrahydrofuran, Cyclohexanone, 1,2-Diethoxyethane, and Acetophenone:	https://www.doi.org/10.1021/je9001976
Solid-Liquid Equilibria of 1,4-Benzenedicarboxylic Acid in Binary Acetic Acid + Water Solvent Mixtures at Elevated Temperatures:	https://www.doi.org/10.1021/je049697k

Legend

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
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume