1,4-Benzenedicarboxaldehyde

Other names:	1,4-Benzenedialdehyde
	1,4-Benzenedicarbaldehyde
	1,4-Diformylbenzene
	4-Formylbenzaldehyde
	NSC 13395
	Terephtaldehyde
	Terephthaladehyde
	Terephthalaldehyde
	Terephthaldialdehyde
	Terephthaldicarboxaldehyde
	p-Benzenedialdehyde
	p-Benzenedicarboxaldehyde
	p-Formylbenzaldehyde
	p-Phthalaldehyde
	p-Phthaldialdehyde
	terephthaldehyde
	terephthalic aldehyde
Inchi:	InChI=1S/C8H6O2/c9-5-7-1-2-8(6-10)4-3-7/h1-6H
InchiKey:	KUCOHFSKRZZVRO-UHFFFAOYSA-N
Formula:	C8H6O2
SMILES:	O=Cc1ccc(C=O)cc1
Mol. weight [g/mol]:	134.13
CAS:	623-27-8

Physical Properties

Property code	Value	Unit	Source
ea	1.28 ± 0.09	eV	NIST Webbook
ea	0.56	eV	NIST Webbook
ea	1.24 ± 0.09	eV	NIST Webbook
gf	-79.78	kJ/mol	Joback Method
hf	-154.55	kJ/mol	Joback Method
hfus	14.71	kJ/mol	Joback Method
hvap	49.78	kJ/mol	Joback Method
ie	10.13 ± 0.01	eV	NIST Webbook
log10ws	-1.95		Crippen Method
logp	1.312		Crippen Method
mcvol	102.960	ml/mol	McGowan Method

pc	4316.89	kPa		Joback Method
rinpol	1166.00			NIST Webbook
ripol	2347.00			NIST Webbook
tb	519.50 ± 1.50	K		NIST Webbook
tb	519.70	K		NIST Webbook
tc	733.14	K		Joback Method
tf	387.25	K		Solubility determination and thermodynamic modelling of terephthaldialdehyde in ten organic solvents from T = (273.15 to 318.15) K and mixing properties of solutions
tf	389.00	K		NIST Webbook
vc	0.409	m3/kmol		Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	208.76	J/mol×K	511.42	Joback Method
cpg	218.33	J/mol×K	548.37	Joback Method
cpg	227.27	J/mol×K	585.33	Joback Method
cpg	235.61	J/mol×K	622.28	Joback Method
cpg	243.38	J/mol×K	659.23	Joback Method
cpg	250.59	J/mol×K	696.19	Joback Method
cpg	257.27	J/mol×K	733.14	Joback Method
dvisc	0.0025093	Pa×s	302.86	Joback Method
dvisc	0.0015427	Pa×s	337.62	Joback Method
dvisc	0.0010385	Pa×s	372.38	Joback Method
dvisc	0.0007480	Pa×s	407.14	Joback Method
dvisc	0.0005673	Pa×s	441.90	Joback Method
dvisc	0.0004480	Pa×s	476.66	Joback Method
dvisc	0.0003653	Pa×s	511.42	Joback Method

Sources

Determination and correlation of terephthaldialdehyde solubility in Determination and Modeling of ethanol, n-propanol, isopropanol acetate, Solid-Liquid Equilibrium for Ternary Solvent Methyl Isophthaldialdehyde Mixed Solvents at temperatures from Hixed solvents for Terephthaldehyde 273 to K to 318.15 K 4-Hydroxybenzaldehyde + Ethyl Acetate/Acetone:

https://www.doi.org/10.1016/j.jct.2016.10.044

https://www.doi.org/10.1021/acs.jced.8b00801

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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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