Terephthalaldehyde

Other names:	1,4-Benzenedialdehyde
	1,4-Benzenedicarbaldehyde
	1,4-Diformylbenzene
	1,4-benzenedicarboxaldehyde
	4-Formylbenzaldehyde
	NSC 13395
	Terephtaldehyde
	Terephthaladehyde
	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

Physical Properties

Property code	Value	Unit	Source
af	0.4808		Cheméo Relay (1.0)
ea	1.24 ± 0.09	eV	NIST Webbook
ea	1.28 ± 0.09	eV	NIST Webbook
ea	0.56	eV	NIST Webbook
gf	-79.78	kJ/mol	Joback Method
hf	-171.47	kJ/mol	Cheméo Relay (1.0)
hfus	14.71	kJ/mol	Joback Method
hvap	68.60	kJ/mol	Cheméo Relay (1.0)
ie	10.13 ± 0.01	eV	NIST Webbook
log10ws	-1.90		Cheméo Relay (1.0)
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	763.74	K	Cheméo Relay (1.0)
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

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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):	
Determination and Modeling of Solid-Liquid Equilibrium for Ternary Systems of Terephthaldialdehyde + 4-Hydroxybenzaldehyde + Ethyl Acetate/Acetone:	https://www.doi.org/10.1021/acs.jced.8b00801

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Solubility determination and thermodynamic modelling of terephthaldialdehyde in ten organic solvents from T = (273.15 to 318.15) K and mixing properties of solutions: https://www.doi.org/10.1016/j.jct.2016.07.013

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C623278&Units=SI

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Cheméo Relay (1.0, beta):

Determination and correlation of terephthaldialdehyde solubility in ethanol, isopropanol, ethyl acetate, isopentanol, N,N-dimethylformamide and N-methyl-2-pyrrolidone from 273.15 K to 318.15 K: https://www.doi.org/10.1016/j.jct.2016.10.044

Solubility of Terephthalaldehyde in N-Methyl-2-pyrrolidone and Solid–Liquid Phase Equilibrium for Ternary Systems of Terephthalic Acid + Terephthaldialdehyde + N,N-Dimethylformamide/N-Methyl-2-pyrrolidone: https://www.doi.org/10.1021/acs.jced.8b00091

Legend

af:	Acentric Factor
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