TEREPHTHALALDEHYDIC ACID

Other names: 4-carboxybenzaldehyde
4-formylbenzoic acid
Terephthaldehydic acid
p-Carboxybenzaldehyde
p-Formylbenzoic acid
terephthaladehydic acid
Inchi: InChI=1S/C8H6O3/c9-5-6-1-3-7(4-2-6)8(10)11/h1-5H,(H,10,11)
InchiKey: GOUHYARYYWKXHS-UHFFFAOYSA-N
Formula: C8H6O3
SMILES: O=Cc1ccc(C(=O)O)cc1
Mol. weight [g/mol]: 150.13

Physical Properties

Property code	Value	Unit	Source
af	0.7163		Cheméo Relay (1.0)
gf	-246.00	kJ/mol	Joback Method
hf	-415.85	kJ/mol	Cheméo Relay (1.0)
hfus	18.10	kJ/mol	Joback Method
hvap	98.09	kJ/mol	Cheméo Relay (1.0)
ie	9.97	eV	Cheméo Relay (1.0)
log10ws	-1.89		Cheméo Relay (1.0)
logp	1.197		Crippen Method
mcvol	108.830	ml/mol	McGowan Method
pc	4815.84	kPa	Joback Method
tb	563.20	K	Cheméo Relay (1.0)
tc	839.94	K	Cheméo Relay (1.0)
tf	471.81	K	Cheméo Relay (1.0)
vc	0.388	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.78	J/mol×K	608.81	Joback Method
cpg	254.76	J/mol×K	643.85	Joback Method

cpg	262.19	J/mol×K	678.89	Joback Method
cpg	269.11	J/mol×K	713.93	Joback Method
cpg	275.53	J/mol×K	748.97	Joback Method
cpg	281.48	J/mol×K	784.01	Joback Method
cpg	286.98	J/mol×K	819.05	Joback Method
dvisc	0.0034418	Pa×s	371.61	Joback Method
dvisc	0.0015021	Pa×s	411.14	Joback Method
dvisc	0.0007582	Pa×s	450.68	Joback Method
dvisc	0.0004273	Pa×s	490.21	Joback Method
dvisc	0.0002624	Pa×s	529.74	Joback Method
dvisc	0.0001724	Pa×s	569.28	Joback Method
dvisc	0.0001196	Pa×s	608.81	Joback Method
hfust	21.30	kJ/mol	452.20	NIST Webbook

Sources

Solid-Liquid Equilibria of Several Systems Containing Acetic Acid: https://www.doi.org/10.1021/je034114c

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

Cheméo Relay (1.0):

Solubilities of 4-Formylbenzoic Acid in Ethanoic Acid, Water, and Ethanoic Acid/Water Mixtures with Different Compositions from (303.2 to 473.2) K: https://www.doi.org/10.1021/je100632c

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

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

Cheméo Relay (1.0, beta):

Determination and modeling of aqueous solubility of 4-position substituted benzoic acid compounds: https://www.doi.org/10.1016/j.fluid.2012.11.023

Solubilities of 4-Carboxybenzaldehyde and 4,4'-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

UC Hall Temperature Solution: http://webbook.nist.gov/cgi/cbook.cgi?ID=C619669&Units=SI

NIST Webbook:

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Solubility Determination, Modeling, and Preferential Solvation of Terephthalaldehydic Acid Dissolvend in Aqueous Solvent Mixtures of Methanol, Ethanol, Isopropanol, and N-Methyl-2-pyrrolidone: https://www.doi.org/10.1021/acs.jced.8b01262

Legend

af: Acentric Factor

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

gf: Standard Gibbs free energy of formation

hf: Enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

hfust: Enthalpy of fusion 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume