4-ACETYLBENZOIC ACID

Other names: Benzoic acid, 4-acetyl-
p-carboxyacetophenone
Inchi: InChI=1S/C9H8O3/c1-6(10)7-2-4-8(5-3-7)9(11)12/h2-5H,1H3,(H,11,12)
InchiKey: QBHDSQZASIBAAI-UHFFFAOYSA-N
Formula: C9H8O3
SMILES: CC(=O)c1ccc(C(=O)O)cc1
Mol. weight [g/mol]: 164.16

Physical Properties

Property code	Value	Unit	Source
af	0.7378		Cheméo Relay (1.0)
gf	-266.98	kJ/mol	Joback Method
hf	-482.16	kJ/mol	Cheméo Relay (1.0)
hfus	20.00	kJ/mol	Joback Method
hvap	101.06	kJ/mol	Cheméo Relay (1.0)
ie	9.77	eV	Cheméo Relay (1.0)
log10ws	-2.07		Cheméo Relay (1.0)
logp	1.587		Crippen Method
mcvol	122.920	ml/mol	McGowan Method
pc	4173.09	kPa	Joback Method
rinpol	1236.00		NIST Webbook
tb	559.54	K	Cheméo Relay (1.0)
tc	809.56	K	Cheméo Relay (1.0)
tf	480.34	K	Cheméo Relay (1.0)
vc	0.444	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.16	J/mol×K	636.90	Joback Method
cpg	337.06	J/mol×K	848.29	Joback Method
cpg	330.78	J/mol×K	813.05	Joback Method
cpg	323.98	J/mol×K	777.82	Joback Method
cpg	316.64	J/mol×K	742.59	Joback Method

cpg	308.74	J/mol×K	707.36	Joback Method
cpg	300.25	J/mol×K	672.13	Joback Method
dvisc	0.0003230	Pa×s	513.86	Joback Method
dvisc	0.0000916	Pa×s	636.90	Joback Method
dvisc	0.0001316	Pa×s	595.88	Joback Method
dvisc	0.0001994	Pa×s	554.87	Joback Method
dvisc	0.0025185	Pa×s	390.81	Joback Method
dvisc	0.0005688	Pa×s	472.84	Joback Method
dvisc	0.0011152	Pa×s	431.82	Joback Method

Sources

Cheméo Relay (1.0, beta):

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C586890&Units=SI

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

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

Cheméo Relay (1.0):

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
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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