

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
CAS:	586-89-0

Physical Properties

Property code	Value	Unit	Source
gf	-266.98	kJ/mol	Joback Method
hf	-381.42	kJ/mol	Joback Method
hfus	20.00	kJ/mol	Joback Method
hvap	68.74	kJ/mol	Joback Method
log10ws	-2.19		Crippen Method
logp	1.587		Crippen Method
mcvol	122.920	ml/mol	McGowan Method
pc	4173.09	kPa	Joback Method
rinpol	1236.00		NIST Webbook
tb	636.90	K	Joback Method
tc	848.29	K	Joback Method
tf	390.81	K	Joback Method
vc	0.463	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.16	J/mol×K	636.90	Joback Method
cpg	300.25	J/mol×K	672.13	Joback Method
cpg	308.74	J/mol×K	707.36	Joback Method
cpg	316.64	J/mol×K	742.59	Joback Method
cpg	323.98	J/mol×K	777.82	Joback Method
cpg	330.78	J/mol×K	813.05	Joback Method

cpg	337.06	J/mol×K	848.29	Joback Method
dvisc	0.0025185	Pa×s	390.81	Joback Method
dvisc	0.0011152	Pa×s	431.82	Joback Method
dvisc	0.0005688	Pa×s	472.84	Joback Method
dvisc	0.0003230	Pa×s	513.86	Joback Method
dvisc	0.0001994	Pa×s	554.87	Joback Method
dvisc	0.0001316	Pa×s	595.88	Joback Method
dvisc	0.0000916	Pa×s	636.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C586890&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
Joback Method	https://en.wikipedia.org/wiki/Joback_method

Legend

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
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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