Benzenepropanoic acid, «alpha»-oxo-

Other names:	Pyruvic acid, phenyl-
	«beta»-Phenylpyruvic acid
	Phenylpyroracemic acid
	Phenylpyruvic acid
	2-Oxo-3-phenylpropanoic acid
	3-Phenyl-2-oxopropanoic acid
	3-Phenylpyruvic acid
	114-76-1 (hydrochloride)
Inchi:	InChI=1S/C9H8O3/c10-8(9(11)12)6-7-4-2-1-3-5-7/h1-5H,6H2,(H,11,12)
InchiKey:	BTNMPGBKDVTSJY-UHFFFAOYSA-N
Formula:	C9H8O3
SMILES:	O=C(O)C(=O)Cc1ccccc1
Mol. weight [g/mol]:	164.16
CAS:	156-06-9

Physical Properties

Property code	Value	Unit	Source
gf	-257.35	kJ/mol	Joback Method
hf	-369.95	kJ/mol	Joback Method
hfus	20.39	kJ/mol	Joback Method
hvap	68.07	kJ/mol	Joback Method
log10ws	-1.07		Crippen Method
logp	0.883		Crippen Method
mcvol	122.920	ml/mol	McGowan Method
pc	4255.16	kPa	Joback Method
tb	631.92	K	Joback Method
tc	842.40	K	Joback Method
tf	378.29	K	Joback Method
vc	0.463	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.62	J/mol×K	631.92	Joback Method

cpg	301.90	J/mol×K	667.00	Joback Method
cpg	310.54	J/mol×K	702.08	Joback Method
cpg	318.55	J/mol×K	737.16	Joback Method
cpg	325.97	J/mol×K	772.24	Joback Method
cpg	332.84	J/mol×K	807.32	Joback Method
cpg	339.17	J/mol×K	842.40	Joback Method
dvisc	0.0034870	Pa×s	378.29	Joback Method
dvisc	0.0014117	Pa×s	420.56	Joback Method
dvisc	0.0006742	Pa×s	462.83	Joback Method
dvisc	0.0003643	Pa×s	505.11	Joback Method
dvisc	0.0002165	Pa×s	547.38	Joback Method
dvisc	0.0001387	Pa×s	589.65	Joback Method
dvisc	0.0000943	Pa×s	631.92	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C156069&Units=SI

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