Benzenepropanoic acid, 4-hydroxy-«alpha»-oxo-

Other names: Pyruvic acid, (p-hydroxyphenyl)-
(p-Hydroxyphenyl)pyruvic acid
Testacid
3-(p-Hydroxyphenyl)-2-oxopropanoic acid
4-Hydroxyphenylpyruvic acid

Inchi: InChI=1S/C9H8O4/c10-7-3-1-6(2-4-7)5-8(11)9(12)13/h1-4,10H,5H2,(H,12,13)

InchiKey: KKADPXVIOXHVKN-UHFFFAOYSA-N

Formula: C9H8O4

SMILES: O=C(O)C(=O)Cc1ccc(O)cc1

Mol. weight [g/mol]: 180.16

CAS: 156-39-8

Physical Properties

Property code	Value	Unit	Source
gf	-411.97	kJ/mol	Joback Method
hf	-547.26	kJ/mol	Joback Method
hfus	26.18	kJ/mol	Joback Method
hvap	81.09	kJ/mol	Joback Method
log10ws	-0.62		Crippen Method
logp	0.588		Crippen Method
mcvol	128.790	ml/mol	McGowan Method
pc	5220.69	kPa	Joback Method
rinpol	1365.00		NIST Webbook
rinpol	1347.00		NIST Webbook
tb	712.54	K	Joback Method
tc	931.70	K	Joback Method
tf	490.01	K	Joback Method
vc	0.428	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.22	J/mol×K	712.54	Joback Method
cpg	340.12	J/mol×K	749.07	Joback Method

cpg	347.50	J/mol×K	785.59	Joback Method
cpg	354.44	J/mol×K	822.12	Joback Method
cpg	361.01	J/mol×K	858.64	Joback Method
cpg	367.27	J/mol×K	895.17	Joback Method
cpg	373.31	J/mol×K	931.70	Joback Method
dvisc	0.0002777	Pa×s	490.01	Joback Method
dvisc	0.0001188	Pa×s	527.10	Joback Method
dvisc	0.0000568	Pa×s	564.19	Joback Method
dvisc	0.0000297	Pa×s	601.28	Joback Method
dvisc	0.0000168	Pa×s	638.36	Joback Method
dvisc	0.0000101	Pa×s	675.45	Joback Method
dvisc	0.0000064	Pa×s	712.54	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C156398&Units=SI
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

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