Benzaldehyde, 3,4-dihydroxy-

Other names:	1,2-Dihydroxy-4-formylbenzene
	3,4-Dihydroxybenzenecarbonal
	3,4-dihydroxybenzaldehyde
	4-Formyl-1,2-benzenediol
	4-Formyl-1,2-dihydroxybenzene
	NC 033
	NSC 22961
	Protocatechualdehyde
	Protocatechuic aldehyde
	Rancinamycin IV
	protocatechoic aldehyde
Inchi:	InChI=1S/C7H6O3/c8-4-5-1-2-6(9)7(10)3-5/h1-4,9-10H
InchiKey:	IBGBGRVKPALMCQ-UHFFFAOYSA-N
Formula:	C7H6O3
SMILES:	O=Cc1ccc(O)c(O)c1
Mol. weight [g/mol]:	138.12
CAS:	139-85-5

Physical Properties

Property code	Value	Unit	Source
gf	-288.29	kJ/mol	Joback Method
hf	-391.48	kJ/mol	Joback Method
hfus	21.78	kJ/mol	Joback Method
hvap	66.20	kJ/mol	Joback Method
log10ws	-0.81		Crippen Method
logp	0.910		Crippen Method
mcvol	99.040	ml/mol	McGowan Method
pc	7097.39	kPa	Joback Method
tb	596.14	K	Joback Method
tc	841.41	K	Joback Method
tf	460.51	K	Joback Method
vc	0.269	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	235.91	J/mol×K	596.14	Joback Method
cpg	268.22	J/mol×K	800.53	Joback Method
cpg	262.52	J/mol×K	759.65	Joback Method
cpg	256.59	J/mol×K	718.78	Joback Method
cpg	250.27	J/mol×K	677.90	Joback Method
cpg	243.43	J/mol×K	637.02	Joback Method
cpg	273.83	J/mol×K	841.41	Joback Method
dvisc	0.0000096	Pa×s	596.14	Joback Method
dvisc	0.0000146	Pa×s	573.53	Joback Method
dvisc	0.0000227	Pa×s	550.93	Joback Method
dvisc	0.0000368	Pa×s	528.33	Joback Method
dvisc	0.0000623	Pa×s	505.72	Joback Method
dvisc	0.0001108	Pa×s	483.12	Joback Method
dvisc	0.0002085	Pa×s	460.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C139855&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamic Difference between Protocatechualdehyde and p-Hydroxybenzaldehyde in Aqueous Sodium Chloride Solutions:	https://www.doi.org/10.1021/acs.jced.6b00458
Solubilities of Protocatechuic Aldehyde, Caffeic Acid, d-Galactose, and d-Rammose Pentahydrate in Ethanol Water Solutions:	https://www.doi.org/10.1021/je300323g
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume