Benzoic acid, 3,4,5-trihydroxy-

Other names:	3,4,5-Trihydroxybenzoic acid
	Gallic acid
	Kyselina 3,4,5-trihydroxybenzoova
	Kyselina gallova
Inchi:	InChI=1S/C7H6O5/c8-4-1-3(7(11)12)2-5(9)6(4)10/h1-2,8-10H,(H,11,12)
InchiKey:	LNTHITQWFMADLM-UHFFFAOYSA-N
Formula:	C7H6O5
SMILES:	O=C(O)c1cc(O)c(O)c(O)c1
Mol. weight [g/mol]:	170.12
CAS:	149-91-7

Physical Properties

Property code	Value	Unit	Source
chs	-2600.00 ± 5.00	kJ/mol	NIST Webbook
gf	-609.13	kJ/mol	Joback Method
hf	-748.02	kJ/mol	Joback Method
hfs	-1013.00 ± 5.00	kJ/mol	NIST Webbook
hfus	30.96	kJ/mol	Joback Method
hvap	95.92	kJ/mol	Joback Method
log10ws	-1.16		Aqueous Solubility Prediction Method
logp	0.502		Crippen Method
mcvol	110.780	ml/mol	McGowan Method
pc	10918.83	kPa	Joback Method
rinpol	1754.00		NIST Webbook
tb	774.15	K	Joback Method
tc	1010.28	K	Joback Method
tf	536.60	K	Thermochemical and structural studies of gallic and ellagic acids
tf	533.15	K	Thermodynamic modeling studies of aqueous solubility of caffeine, gallic acid and their cocrystal in the temperature range of 303 K-363 K
vc	0.242	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	339.13	J/mol×K	1010.28	Joback Method
cpg	299.19	J/mol×K	774.15	Joback Method
cpg	304.89	J/mol×K	813.51	Joback Method
cpg	310.73	J/mol×K	852.86	Joback Method
cpg	316.89	J/mol×K	892.22	Joback Method
cpg	323.55	J/mol×K	931.57	Joback Method
cpg	330.91	J/mol×K	970.93	Joback Method
dvisc	2.2764543e-08	Pa×s	774.15	Joback Method
dvisc	0.0000004	Pa×s	640.98	Joback Method
dvisc	0.0000002	Pa×s	663.17	Joback Method
dvisc	0.0000001	Pa×s	685.37	Joback Method
dvisc	8.1649065e-08	Pa×s	707.57	Joback Method
dvisc	5.1976473e-08	Pa×s	729.76	Joback Method
dvisc	3.3981406e-08	Pa×s	751.95	Joback Method
hsubt	75.10	kJ/mol	406.00	NIST Webbook

Sources

Solubility of Gallic Acid in Methanol, Ethanol, Water, and Ethyl Acetate:	https://www.doi.org/10.1021/je700633w
Binary diffusion coefficients of phenolic compounds in subcritical water using a chromatographic peak broadening technique:	https://www.doi.org/10.1016/j.fluid.2010.12.003
Solubilities of Gallic Acid and Its Esters in Water:	https://www.doi.org/10.1021/je0601661
Solubility of Gallic Acid, Catechin, and Protocatechuic Acid in Subcritical Water from (298.79 to 419.65) K:	https://www.doi.org/10.1021/je901097n
Thermochemical and structural studies of gallic and ellagic acids:	https://www.doi.org/10.1016/j.jct.2018.09.027
Differential Scanning Calorimetry Data and Solubility of Rosmarinic Acid in Different Pure Solvents and in Binary Mixtures (Methyl Acetate + Water) and (Ethyl Acetate + Water) from 298.2 to 318.2 K:	https://www.doi.org/10.1021/acs.jced.6b00008
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Solubility of Veratric Acid in Eight Monosolvents and Ethanol + 1-Butanol at Various Temperatures:	https://www.doi.org/10.1021/je400029t
Solubility of Gallic Acid, Vanillin, Syringic Acid, and Protocatechuic Acid in Aqueous Sulfate Solutions from (298.15 to 318.15) K:	https://www.doi.org/10.1021/je800205e
Temperature and salt addition effects on the solubility behaviour of some phenolic compounds in water:	https://www.doi.org/10.1016/j.jct.2006.06.014
Solubility of gallic acid in liquid mixtures of (ethanol + water) from (293.15 to 318.15) K:	https://www.doi.org/10.1016/j.jct.2012.06.022
Joback Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C149917&Units=SI
Thermodynamic modeling studies of aqueous solubility of caffeine, gallic acid and their cocrystal in the temperature range of 303 K-363 K:	https://www.doi.org/10.1016/j.fluid.2017.09.021
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=980
Reactive Extraction of Gallic Acid Using Tributyl Phosphate in Different Classes of Diluents:	https://www.doi.org/10.1021/acs.jced.9b00192

Solubility of the Natural Antioxidant Gallic Acid in Supercritical CO2 + Ethanol as a Cosolvent:	https://www.doi.org/10.1021/je060273v
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Solubility of some phenolic compounds in aqueous alkali metal nitrate solutions from (293.15 to 318.15) K:	https://www.doi.org/10.1016/j.jct.2008.06.006

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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