Benzoic acid, 2,3-dihydroxy-

Other names:	2,3 DHB
	2,3-dihydroxybenzoic acid
	3-Hydroxysalicylic acid
	Catechol-3-carboxylic acid
	DOBK
	Pyrocatechuic acid
	o-Pyrocatechuic acid
Inchi:	InChI=1S/C7H6O4/c8-5-3-1-2-4(6(5)9)7(10)11/h1-3,8-9H,(H,10,11)
InchiKey:	GLDQAMYCGOIJDV-UHFFFAOYSA-N
Formula:	C7H6O4
SMILES:	O=C(O)c1cccc(O)c1O
Mol. weight [g/mol]:	154.12
CAS:	303-38-8

Physical Properties

Property code	Value	Unit	Source
gf	-454.51	kJ/mol	Joback Method
hf	-570.71	kJ/mol	Joback Method
hfus	31.90	kJ/mol	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
hsub	110.70 ± 0.80	kJ/mol	NIST Webbook
hvap	82.90	kJ/mol	Joback Method
log10ws	-0.63		Crippen Method
logp	0.796		Crippen Method
mcvol	104.910	ml/mol	McGowan Method
pc	8175.04	kPa	Joback Method
rinpol	1372.00		NIST Webbook
tb	693.53	K	Joback Method
tc	922.45	K	Joback Method
tf	529.26	K	Joback Method
vc	0.277	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	296.25	J/mol×K	884.30	Joback Method
cpg	290.73	J/mol×K	846.15	Joback Method
cpg	285.24	J/mol×K	807.99	Joback Method
cpg	279.67	J/mol×K	769.84	Joback Method
cpg	273.90	J/mol×K	731.68	Joback Method
cpg	267.80	J/mol×K	693.53	Joback Method
cpg	301.93	J/mol×K	922.45	Joback Method
dvisc	0.0000285	Pa×s	529.26	Joback Method
dvisc	0.0000008	Pa×s	693.53	Joback Method
dvisc	0.0000013	Pa×s	666.15	Joback Method
dvisc	0.0000021	Pa×s	638.77	Joback Method
dvisc	0.0000038	Pa×s	611.39	Joback Method
dvisc	0.0000069	Pa×s	584.02	Joback Method
dvisc	0.0000136	Pa×s	556.64	Joback Method
hfust	31.90	kJ/mol	476.60	NIST Webbook
hsubt	109.10 ± 0.80	kJ/mol	354.00	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers: https://www.doi.org/10.1021/je900777q

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=C303388&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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