«beta»-Resorcylic acid

Other names:	.beta.-resorcinolic acid
	.beta.-resorcylic acid
	2,4-Dhba
	2,4-dihydroxybenzoic acid
	4-carboxyresorcinol
	4-hydroxysalicylic acid
	BRA
	Coupler 320
	NSC 13564
	Resorcylic acid, «beta»
	benzoic acid, 2,4-dihydroxy-
	p-hydroxysalicylic acid
	«beta»-Resorcinolic acid
Inchi:	InChI=1S/C7H6O4/c8-4-1-2-5(7(10)11)6(9)3-4/h1-3,8-9H,(H,10,11)
InchiKey:	UIAFKZKHHVMJGS-UHFFFAOYSA-N
Formula:	C7H6O4
SMILES:	O=C(O)c1ccc(O)cc1O
Mol. weight [g/mol]:	154.12
CAS:	89-86-1

Physical Properties

Property code	Value	Unit	Source
gf	-454.51	kJ/mol	Joback Method
hf	-570.71	kJ/mol	Joback Method
hfus	31.00	kJ/mol	Thermochemical study of 2,4-, 2,6- and 3,4-dihydroxybenzoic acids in the liquid phase using a TG apparatus
hsub	126.40 ± 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	1532.00		NIST Webbook
rinpol	1532.00		NIST Webbook
tb	693.53	K	Joback Method

tc	922.45	K	Joback Method
tf	492.00 ± 4.00	K	NIST Webbook
vc	0.277	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.80	J/mol×K	693.53	Joback Method
cpg	273.90	J/mol×K	731.68	Joback Method
cpg	279.67	J/mol×K	769.84	Joback Method
cpg	285.24	J/mol×K	807.99	Joback Method
cpg	290.73	J/mol×K	846.15	Joback Method
cpg	296.25	J/mol×K	884.30	Joback Method
cpg	301.93	J/mol×K	922.45	Joback Method
dvisc	0.0000285	Pa×s	529.26	Joback Method
dvisc	0.0000136	Pa×s	556.64	Joback Method
dvisc	0.0000069	Pa×s	584.02	Joback Method
dvisc	0.0000038	Pa×s	611.39	Joback Method
dvisc	0.0000021	Pa×s	638.77	Joback Method
dvisc	0.0000013	Pa×s	666.15	Joback Method
dvisc	0.0000008	Pa×s	693.53	Joback Method
hsubt	124.00 ± 0.80	kJ/mol	384.00	NIST Webbook
psub	2.60e-04	kPa	379.13	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	1.92e-04	kPa	376.22	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	1.95e-04	kPa	376.22	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	2.24e-04	kPa	377.32	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers

psub	2.17e-04	kPa	377.32	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	2.20e-04	kPa	377.32	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	2.69e-04	kPa	379.13	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	1.98e-04	kPa	376.22	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	2.64e-04	kPa	379.13	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	3.32e-04	kPa	381.15	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	3.15e-04	kPa	381.15	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	3.19e-04	kPa	381.15	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	3.99e-04	kPa	383.13	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	3.88e-04	kPa	383.13	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers

psub	3.90e-04	kPa	383.13	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	5.01e-04	kPa	385.12	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	4.89e-04	kPa	385.12	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	4.93e-04	kPa	385.12	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	6.13e-04	kPa	387.17	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	5.91e-04	kPa	387.17	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	5.93e-04	kPa	387.17	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	7.62e-04	kPa	389.35	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	7.32e-04	kPa	389.35	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	7.41e-04	kPa	389.35	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers

psub	9.16e-04	kPa	391.30	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	8.84e-04	kPa	391.30	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	8.93e-04	kPa	391.30	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	9.88e-04	kPa	392.11	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	9.61e-04	kPa	392.11	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	9.55e-04	kPa	392.11	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C89861&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermochemical study of 2,4-, 2,6- and 3,4-dihydroxybenzoic acids in the liquid phase using a TG apparatus:	https://www.doi.org/10.1016/j.tca.2011.01.001
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

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
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
psub:	Sublimation pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume