Benzoic acid, 3,5-dihydroxy-

Other names:	3,5-dihydroxybenzoic acid
	5-Carboxyresorcinol
	«alpha»-Resorcylic acid
Inchi:	InChI=1S/C7H6O4/c8-5-1-4(7(10)11)2-6(9)3-5/h1-3,8-9H,(H,10,11)
InchiKey:	UYEMGAFJOZZIFP-UHFFFAOYSA-N
Formula:	C7H6O4
SMILES:	O=C(O)c1cc(O)cc(O)c1
Mol. weight [g/mol]:	154.12
CAS:	99-10-5

Physical Properties

Property code	Value	Unit	Source
gf	-454.51	kJ/mol	Joback Method
hf	-570.71	kJ/mol	Joback Method
hfus	38.30	kJ/mol	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
hsub	143.20 ± 1.80	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	1617.00		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	301.93	J/mol×K	922.45	Joback Method

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
dvisc	0.0000008	Pa×s	693.53	Joback Method
dvisc	0.0000013	Pa×s	666.15	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
hfust	38.30	kJ/mol	508.30	NIST Webbook
hsubt	139.80 ± 1.80	kJ/mol	354.00	NIST Webbook

Sources

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=C99105&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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

Latest version available from:

https://www.chemeo.com/cid/43-065-2/Benzoic-acid-3-5-dihydroxy.pdf

Generated by Cheméo on 2024-10-12 03:19:38.965539738 +0000 UTC m=+3284041.602508986.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.