

Benzoic acid, 2-hydroxy-5-sulfo-

Other names:	2-Hydroxy-5-sulfobenzoic acid 2-Hydroxybenzoic-5-sulfonic acid 3-Carboxy-4-hydroxybenzenesulfonic acid 5-Sulfosalicylic acid 5-Sulphosalicylic acid Benzoic acid, 2-hydroxysulfo- NSC 190565 Salicylic acid, 5-sulfo- Salicylic acid, sulfo- Salicylsulfonic acid Sulfosalicylic acid Sulphosalicylic acid
Inchi:	InChI=1S/C7H6O6S/c8-6-2-1-4(14(11,12)13)3-5(6)7(9)10/h1-3,8H,(H,9,10)(H,11,12,13)
InchiKey:	YCPXWRQRBFJBPZ-UHFFFAOYSA-N
Formula:	C7H6O6S
SMILES:	O=C(O)c1cc(S(=O)(=O)O)ccc1O
Mol. weight [g/mol]:	218.18
CAS:	97-05-2

Physical Properties

Property code	Value	Unit	Source
gf	-914.88	kJ/mol	Joback Method
hf	-1010.45	kJ/mol	Joback Method
hfus	34.47	kJ/mol	Joback Method
hvap	105.87	kJ/mol	Joback Method
log10ws	-0.67		Crippen Method
logp	0.337		Crippen Method
mcvol	133.000	ml/mol	McGowan Method
pc	9555.40	kPa	Joback Method
rinpol	1265.00		NIST Webbook
rinpol	1265.00		NIST Webbook
tb	757.85	K	Joback Method
tc	959.53	K	Joback Method
tf	529.44	K	Joback Method
vc	0.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.55	J/molxK	757.85	Joback Method
cpg	348.46	J/molxK	791.46	Joback Method
cpg	353.95	J/molxK	825.08	Joback Method
cpg	359.04	J/molxK	858.69	Joback Method
cpg	363.77	J/molxK	892.30	Joback Method
cpg	368.18	J/molxK	925.92	Joback Method
cpg	372.29	J/molxK	959.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C97052&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Volumetric approach to the interaction of diglycine in aqueous solutions of	https://www.doi.org/10.1016/j.fluid.2012.08.001
Mixing Solubilities of 25 Sulfonolysis	https://www.doi.org/10.1021/je700159k
Acid and p-Aminobenzoic Acid in Supercritical Carbon Dioxide:	https://en.wikipedia.org/wiki/Joback_method
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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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