

# BENZENESULFONIC ACID

**Other names:** Benzenemonosulfonic acid; Benzenesulphonic acid; Besylic acid; Kyselina benzensulfonova; Phenylsulfonic acid.

**InChI:** InChI=1S/C6H6O3S/c7-10(8,9)6-4-2-1-3-5-6/h1-5H,(H,7,8,9)

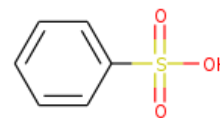
**InChI Key:** SRSXLGNVWSONIS-UHFFFAOYSA-N

**Formula:** C6H6O3S

**SMILES:** O=S(=O)(O)c1ccccc1

**Molecular Weight:** 158.18

**CAS:** 98-11-3



## Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-493.31	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-536.22	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	20.80	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	66.54	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	0.933		Crippen Method
$P_c$	6762.90	kPa	Joback Method
$T_{\text{boil}}$	503.32	K	Joback Method
$T_c$	699.94	K	Joback Method
$T_{\text{fus}}$	283.18	K	Joback Method
$V_c$	0.408	m <sup>3</sup> /kg-mol	Joback Method

## Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	213.65	J/mol×K	503.32	Joback Method

## Sources

**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**NIST Webbook:**

[http://webbook.nist.gov/cgi/inchi/InChI=1S/C6H6O3S/c7-10\(8,9\)6-4-2-1-3-5-6/h1-5H,\(H,7,8,9\)](http://webbook.nist.gov/cgi/inchi/InChI=1S/C6H6O3S/c7-10(8,9)6-4-2-1-3-5-6/h1-5H,(H,7,8,9))

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

$C_{p, gas}$ : Ideal gas heat capacity (J/mol×K).

$\Delta_f G^\circ$ : Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{gas}$ : Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{fus} H^\circ$ : Enthalpy of fusion at standard conditions (kJ/mol).

$\Delta_{vap} H^\circ$ : Enthalpy of vaporization at standard conditions (kJ/mol).

$\log P_{oct/wat}$ : Octanol/Water partition coefficient .

$P_c$ : Critical Pressure (kPa).

$T_{boil}$ : Normal Boiling Point Temperature (K).

$T_c$ : Critical Temperature (K).

$T_{fus}$ : Normal melting (fusion) point (K).

$V_c$ : Critical Volume (m<sup>3</sup>/kg-mol).

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