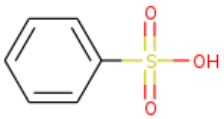
BENZENESULFONIC ACID

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
$\Delta_f G°$	-493.31	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-536.22	kJ/mol	Joback Method
$\Delta_{fus} H°$	20.80	kJ/mol	Joback Method
$\Delta_{vap} H°$	66.54	kJ/mol	Joback Method
$logP_{oct/wat}$	0.933		Crippen Method
P_c	6762.90	kPa	Joback Method
T_{boil}	503.32	K	Joback Method
T_c	699.94	K	Joback Method
T_{fus}	283.18	K	Joback Method
V_c	0.408	m^3/kg-mol	Joback Method

Temperature Dependent Properties

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

Sources

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

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
$\mathbf{\Delta_f G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\mathbf{\Delta_f H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\mathbf{\Delta_{fus} H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\mathbf{\Delta_{vap} H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\mathbf{\mathit{log}P_{oct/wat}}$: Octanol/Water partition coefficient .
$\mathbf{P_c}$: Critical Pressure (kPa).
$\mathbf{T_{boil}}$: Normal Boiling Point Temperature (K).
$\mathbf{T_c}$: Critical Temperature (K).
$\mathbf{T_{fus}}$: Normal melting (fusion) point (K).
$\mathbf{V_c}$: Critical Volume (m^3/kg-mol).