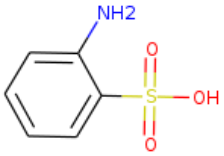
Aniline-o-sulfonic acid

Other names: 1-Aminobenzene-2-sulfonic acid; 2-Aminobenzenesulfonic acid; 2-Aminobenzenesulphonic acid; Aniline-2-sulfonic acid; Aniline-o-sulphonic acid; Anilino-2-sulfonic acid; Anilino-o-sulfonic acid; Anilino-o-sulphonic acid; Benzenesulfonic acid, 2-amino-; Benzenesulfonic acid, o-amino-; NSC 147; Orthanilic acid; o-Aminobenzenesulfonic acid; o-Aminophenylsulfonic acid; o-Sulfanilic acid.



InChI: InChI=1S/C6H7NO3S/c7-5-3-1-2-4-6(5)11(8,9)10/h1-4H,7H2,(H,8,9,10)

InChI Key: ZMCHBSMFKQYNKA-UHFFFAOYSA-N

Formula: C6H7NO3S

SMILES: Nc1ccccc1S(=O)(=O)O

Molecular Weight: 173.19

CAS: 88-21-1

Physical Properties

Property	Value	Unit	Source
$\Delta_c H°_{solid}$	-3363.90 ± 0.60	kJ/mol	NIST Webbook
$\Delta_f G°$	-436.49	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-513.90	kJ/mol	Joback Method
$\Delta_f H°_{solid}$	-559.60 ± 1.10	kJ/mol	NIST Webbook
$\Delta_{fus} H°$	25.61	kJ/mol	Joback Method
$\Delta_{vap} H°$	77.84	kJ/mol	Joback Method
$logP_{oct/wat}$	0.516		Crippen Method
P_c	7255.44	kPa	Joback Method
T_{boil}	580.83	K	Joback Method
T_c	787.92	K	Joback Method
T_{fus}	378.96	K	Joback Method
V_c	0.438	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	261.80	J/mol×K	580.83	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C6H7NO3S/c7-5-3-1-2-4-6(5)11(8,9)10/h1-4H,7H2,(H,8,9,10)
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\Delta_c H°_{solid}$: Standard solid enthalpy of combustion (kJ/mol).
$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).
$\Delta_f G°$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f H°_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_f H°_{solid}$: Solid phase enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus} H°$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap} H°$: Enthalpy of vaporization at standard conditions (kJ/mol).
$logP_{oct/wat}$: 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^3/kg-mol).