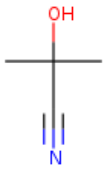
Propanenitrile, 2-hydroxy-2-methyl-

Other names: 2-Cyano-2-hydroxypropane; 2-Cyano-2-propanol; 2-Cyanopropan-2-ol; 2-Hydroxy-2-methylpropanenitrile; 2-Hydroxy-2-methylpropionitrile; 2-Hydroxyisobutyronitrile; 2-Methyllactonitrile; 2-Propanone, cyanohydrin; Acetoncianhidrinei; Acetoncianidrina; Acetoncyaanhydrine; Acetoncyanhydrin; Acetone cyanhydrin; Acetonecyanhydrine; Acetonkyanhydrin; Cyanhydrine d'acetone; Lactonitrile, 2-methyl-; NSC 131093; Propanenitrile, 2-hydroxy-2-methyl-; Rcra waste number P069; UN 1541; USAF RH-8; «alpha»-Hydroxyisobutyronitrile.



InChI: InChI=1S/C4H7NO/c1-4(2,6)3-5/h6H,1-2H3

InChI Key: MWFMGBPGAXYFAR-UHFFFAOYSA-N

Formula: C4H7NO

SMILES: CC(C)(O)C#N

Molecular Weight: 85.10

CAS: 75-86-5

Physical Properties

Property	Value	Unit	Source
$\Delta_c H°_{liquid}$	-2450.60 ± 0.80	kJ/mol	NIST Webbook
$\Delta_f G°$	-18.00	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-121.99	kJ/mol	Joback Method
$\Delta_f H°_{liquid}$	-120.90 ± 0.80	kJ/mol	NIST Webbook
$\Delta_{fus} H°$	4.30	kJ/mol	Joback Method
$\Delta_{vap} H°$	50.36	kJ/mol	Joback Method
IE	11.09	eV	NIST Webbook
$logP_{oct/wat}$	0.281		Crippen Method
P_c	4351.13	kPa	Joback Method
T_{boil}	355.20	K	NIST Webbook
T_c	677.00	K	Joback Method
T_{fus}	251.90 ± 0.60	K	NIST Webbook
V_c	0.293	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	155.39	J/mol×K	481.95	Joback Method
$\Delta_{vap}H$	106.50	kJ/mol	374.0	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C4H7NO/c1-4(2,6)3-5/h6H,1-2H3
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\Delta_c H°_{liquid}$: Standard liquid 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).
$\Delta_f H°_{liquid}$: Liquid 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).
$\Delta_{vap} H$: Enthalpy of vaporization at a given temperature (kJ/mol).
IE: Ionization energy (eV).
$logP_{oct/wat}$: 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).