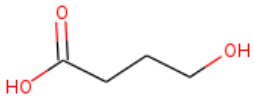
4-Hydroxybutyric acid

Other names: 4-Hydroxybutyric acid; GHB; «gamma»-Hydroxybutyric acid decomposition product.
InChI: InChI=1S/C4H8O3/c5-3-1-2-4(6)7/h5H,1-3H2,(H,6,7)
InChI Key: SJZRECIVHVDYJC-UHFFFAOYSA-N
Formula: C4H8O3
SMILES: O=C(O)CCCO
Molecular Weight: 104.10
CAS: 591-81-1



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-419.76	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-542.93	kJ/mol	Joback Method
$\Delta_f H°_{liquid}$	-710.00 ± 3.00	kJ/mol	NIST Webbook
$\Delta_{fus} H°$	15.89	kJ/mol	Joback Method
$\Delta_{vap} H°$	64.60	kJ/mol	Joback Method
$logP_{oct/wat}$	-0.156		Crippen Method
P_c	5446.55	kPa	Joback Method
T_{boil}	529.15	K	Joback Method
T_c	696.80	K	Joback Method
T_{fus}	306.41	K	Joback Method
V_c	0.303	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	182.35	J/mol×K	529.15	Joback Method
η	0.0000865	Pa×s	529.15	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C4H8O3/c5-3-1-2-4(6)7/h5H,1-3H2,(H,6,7)
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
η: Dynamic viscosity (Pa×s).
$\Delta_f\mathbf{G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f\mathbf{H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_f\mathbf{H°_{liquid}}$: Liquid phase enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus}\mathbf{H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap}\mathbf{H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\boldsymbol{log}\mathbf{P_{oct/wat}}$: 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).