

# 4-Heptyn-3-ol

**InChI:** InChI=1S/C7H12O/c1-3-5-6-7(8)4-2/h7-8H,3-4H2,1-2H3

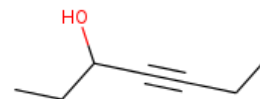
**InChI Key:** FMOKAMXPKGORIR-UHFFFAOYSA-N

**Formula:** C7H12O

**SMILES:** CCC#CC(O)CC

**Molecular Weight:** 112.17

**CAS:** 32398-69-9



## Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	71.60	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-73.02	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	17.57	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	49.62	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	1.171		Crippen Method
$P_c$	3763.78	kPa	Joback Method
$T_{\text{boil}}$	368.00	K	NIST Webbook
$T_c$	645.47	K	Joback Method
$T_{\text{fus}}$	320.57	K	Joback Method
$V_c$	0.403	m <sup>3</sup> /kg-mol	Joback Method

## Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	217.62	J/mol×K	460.3	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/C7H12O/c1-3-5-6-7\(8\)4-2/h7-8H,3-4H2,1-2H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C7H12O/c1-3-5-6-7(8)4-2/h7-8H,3-4H2,1-2H3)

**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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