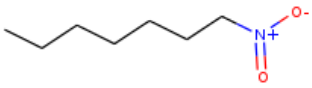
Heptane, 1-nitro-

Other names: 1-Nitroheptane.
InChI: InChI=1S/C7H15NO2/c1-2-3-4-5-6-7-8(9)10/h2-7H2,1H3
InChI Key: UZONFOPDCXAZND-UHFFFAOYSA-N
Formula: C7H15NO2
SMILES: CCCCCCC[N+](=O)[O-]
Molecular Weight: 145.20
CAS: 693-39-0



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	43.61	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-198.57	kJ/mol	Joback Method
$\Delta_{fus} H°$	25.25	kJ/mol	Joback Method
$\Delta_{vap} H°$	47.77	kJ/mol	Joback Method
$logP_{oct/wat}$	2.234		Crippen Method
P_c	2835.36	kPa	Joback Method
T_{boil}	511.40	K	Joback Method
T_c	710.38	K	Joback Method
T_{fus}	312.26	K	Joback Method
V_c	0.509	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	293.28	J/mol×K	511.4	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C7H15NO2/c1-2-3-4-5-6-7-8(9)10/h2-7H2,1H3
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).