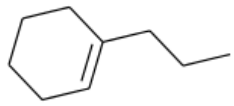
Cyclohexene,1-propyl-

Other names: 1-Propyl-1-cyclohexene; 1-Propylcyclohexene-1.
InChI: InChI=1S/C9H16/c1-2-6-9-7-4-3-5-8-9/h7H,2-6,8H2,1H3
InChI Key: WCPWJMLXSZIWOP-UHFFFAOYSA-N
Formula: C9H16
SMILES: CCCC1=CCCCC1
Molecular Weight: 124.22
CAS: 2539-75-5



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	77.39	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-108.12	kJ/mol	Joback Method
$\Delta_{fus} H°$	10.66	kJ/mol	Joback Method
$\Delta_{vap} H°$	37.32	kJ/mol	Joback Method
IE	8.43 ± 0.01	eV	NIST Webbook
$log P_{oct/wat}$	3.29		Crippen Method
P_c	3009.03	kPa	Joback Method
T_{boil}	429.40 ± 5.00	K	NIST Webbook
T_{boil}	427.20 ± 4.00	K	NIST Webbook
T_c	636.54	K	Joback Method
T_{fus}	216.09	K	Joback Method
V_c	0.46	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	243.01	J/mol×K	433.68	Joback Method

Property	Value	Unit	Temperature (K)	Source
η	0.00	Pa×s	433.68	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:
http://webbook.nist.gov/cgi/inchi/InChI=1S/C9H16/c1-2-6-9-7-4-3-5-8-9/h7H,2-6,8H2,1H3
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).
η: Dynamic viscosity (Pa×s).
Δ_f**G°**: Standard Gibbs free energy of formation (kJ/mol).
Δ_f**H°**$_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
Δ_{fus}**H°**: Enthalpy of fusion at standard conditions (kJ/mol).
Δ_{vap}**H°**: Enthalpy of vaporization at standard conditions (kJ/mol).
IE: Ionization energy (eV).
***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^3/kg-mol).

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