6-Methyl-1,2,3,4-tetrahydroquinoline

Other names: 1,2,3,4-Tetrahydro-6-methylquinoline; Civettal; Quinoline, 1,2,3,4-tetrahydro-6-methyl-.

InChI: InChI=1S/C10H13N/c1-8-4-5-10-9(7-8)3-2-6-11-10/h4-5,7,11H,2-3,6H2,1H3

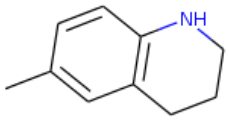
InChI Key: XOKMRXSMOHCNIX-UHFFFAOYSA-N

Formula: C10H13N

SMILES: Cc1ccc2c(c1)CCCN2

Molecular Weight: 147.22

CAS: 91-61-2



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	270.54	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	88.65	kJ/mol	Joback Method
$\Delta_{fus} H°$	19.47	kJ/mol	Joback Method
$\Delta_{vap} H°$	48.61	kJ/mol	Joback Method
$logP_{oct/wat}$	2.35		Crippen Method
P_c	3611.55	kPa	Joback Method
T_{boil}	529.07	K	Joback Method
T_c	768.20	K	Joback Method
T_{fus}	377.61	K	Joback Method
V_c	0.47	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	283.67	J/mol×K	529.07	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C10H13N/c1-8-4-5-10-9(7-8)3-2-6-11-10/h4-5,7,11H,2-3,6H2,1H3

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).

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