

6-ethyl-1,2,3,4,5,6-hexahydro-7H-cyclopenta[b]pyridin-7-one

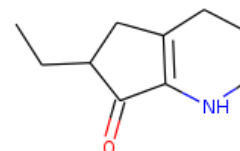
InChI: InChI=1S/C10H15NO/c1-2-7-6-8-4-3-5-11-9(8)10(7)12/h7,11H,2-6H2,1H3

InChI Key: GOTCNQZLHJWEAK-UHFFFAOYSA-N

Formula: C10H15NO

SMILES: CCC1CC2=C(NCCC2)C1=O

Molecular Weight: 165.23



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	102.05	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-167.32	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	20.10	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	51.13	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	1.623		Crippen Method
P_c	3287.81	kPa	Joback Method
T_{boil}	584.65	K	Joback Method
T_c	823.82	K	Joback Method
T_{fus}	431.07	K	Joback Method
V_c	0.516	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	351.21	J/mol×K	584.65	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C10H15NO/c1-2-7-6-8-4-3-5-11-9\(8\)10\(7\)12/h7,11H,2-6H2,1H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C10H15NO/c1-2-7-6-8-4-3-5-11-9(8)10(7)12/h7,11H,2-6H2,1H3)

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).

$logP_{oct/wat}$: 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 (m³/kg-mol).

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