

Pinonaldehyde

Other names: 3-Acetyl-2,2-dimethylcyclobutaneacetaldehyde (pinonaldehyde).

InChI: InChI=1S/C10H16O2/c1-7(12)9-6-8(4-5-11)10(9,2)3/h5,8-9H,4,6H,2,1-3H3

InChI Key: GCHDWVBHKDJOKU-UHFFFAOYSA-N

Formula: C10H16O2

SMILES: CC(=O)C1CC(CC=O)C1(C)C

Molecular Weight: 168.23

CAS: 2704-78-1



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-167.38	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-406.69	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	17.42	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	49.64	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	1.83		Crippen Method
P_c	2749.78	kPa	Joback Method
T_{boil}	532.64	K	Joback Method
T_c	737.03	K	Joback Method
T_{fus}	324.23	K	Joback Method
V_c	0.56	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	353.49	J/mol×K	532.64	Joback Method
$\Delta_{\text{vap}} H$	75.50 ± 5.60	kJ/mol	295.5	NIST Webbook

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C10H16O2/c1-7\(12\)9-6-8\(4-5-11\)10\(9,2\)3/h5,8-9H,4,6H2,1-3H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C10H16O2/c1-7(12)9-6-8(4-5-11)10(9,2)3/h5,8-9H,4,6H2,1-3H3)

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).

$\Delta_{vap} H$: Enthalpy of vaporization at a given temperature (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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