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,4,6H2,1-3H3

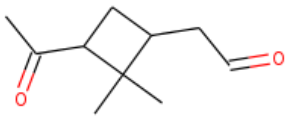
InChI Key: GCHDWVBHKDJOKU-UHFFFAOYSA-N

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
$\Delta_f G°$	-167.38	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-406.69	kJ/mol	Joback Method
$\Delta_{fus} H°$	17.42	kJ/mol	Joback Method
$\Delta_{vap} H°$	49.64	kJ/mol	Joback Method
$logP_{oct/wat}$	1.827		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	0.564	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	353.49	J/mol×K	532.64	Joback Method
$\Delta_{vap} H$	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
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
$\Delta_f\mathbf{G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f\mathbf{H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus}\mathbf{H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap}\mathbf{H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\Delta_{vap}\mathbf{H}$: Enthalpy of vaporization at a given temperature (kJ/mol).
$\boldsymbol{log}\mathbf{P_{oct/wat}}$: 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).