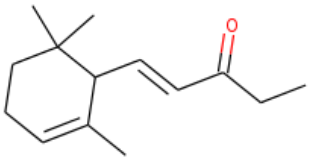
1-Penten-3-one, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)-

Other names: 1-(2,6,6-Trimethylcyclohex-2-en-1-yl)-1-pentene-3-one; 1-(2,6,6-Trimethylcyclohex-2-en-1-yl)pent-1-en-3-one; 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)pent-1-en-3-one; «alpha»-N-Methyl ionone.



InChI: InChI=1S/C14H22O/c1-5-12(15)8-9-13-11(2)7-6-10-14(13,3)4/h7-9,13H,5-6,10H2,1-4H3/b9-8+

InChI Key: VPKMGDRERYMTJX-CMDGGOBGSA-N

Formula: C14H22O

SMILES: CCC(=O)C=CC1C(C)=CCCC1(C)C

Molecular Weight: 206.32

CAS: 7779-30-8

Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	49.88	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-232.12	kJ/mol	Joback Method
$\Delta_{fus} H°$	21.26	kJ/mol	Joback Method
$\Delta_{vap} H°$	53.39	kJ/mol	Joback Method
$log P_{oct/wat}$	3.904		Crippen Method
P_c	2049.31	kPa	Joback Method
T_{boil}	597.01	K	Joback Method
T_c	811.30	K	Joback Method
T_{fus}	332.71	K	Joback Method
V_c	0.722	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	489.29	J/mol×K	597.01	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C14H22O/c1-5-12(15)8-9-13-11(2)7-6-10-14(13,3)4/h7-9,13H,5-6,10H2,1-4H3/b9-8+

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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