

# Octanoic acid, 2-methyl-

**Other names:** 2-Methyloctanoic acid; Caprylic acid, «alpha»-methyl-

**InChI:** InChI=1S/C9H18O2/c1-3-4-5-6-7-8(2)9(10)11/h8H,3-7H2,1-2H3,(H,10,11)

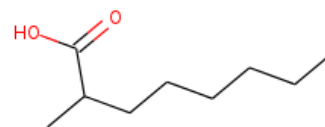
**InChI Key:** YSEQNZOXHCKLOG-UHFFFAOYSA-N

**Formula:** C<sub>9</sub>H<sub>18</sub>O<sub>2</sub>

**SMILES:** CCCCCC(C)C(=O)O

**Molecular Weight:** 158.24

**CAS:** 3004-93-1



## Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-243.28	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-499.18	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	21.23	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	58.66	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	2.68		Crippen Method
$P_c$	2715.50	kPa	Joback Method
$T_{\text{boil}}$	550.93	K	Joback Method
$T_c$	721.77	K	Joback Method
$T_{\text{fus}}$	286.94	K	Joback Method
$V_c$	0.56	m <sup>3</sup> /kg-mol	Joback Method

## Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	355.57	J/mol×K	550.93	Joback Method
$\eta$	0.00	Paxs	550.93	Joback Method

## Sources

**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**NIST Webbook:** [http://webbook.nist.gov/cgi/inchi/InChI=1S/C9H18O2/c1-3-4-5-6-7-8\(2\)9\(10\)11/h8H,3-7H,2,1-2H3,\(H,10,11\)](http://webbook.nist.gov/cgi/inchi/InChI=1S/C9H18O2/c1-3-4-5-6-7-8(2)9(10)11/h8H,3-7H,2,1-2H3,(H,10,11))

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

$C_{p,gas}$ : Ideal gas heat capacity (J/molxK).

$\eta$ : Dynamic viscosity (Pa $\times$ s).

$\Delta_f G^\circ$ : 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 (m<sup>3</sup>/kg-mol).

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