

2,4-Dimethylpentane-2,4-diol

Other names: 2,4-Dimethylpentane-2,4-diol.

InChI: InChI=1S/C7H16O2/c1-6(2,8)5-7(3,4)9/h8-9H,5H2,1-4H3

InChI Key: DBTGFWMBFZBBEF-UHFFFAOYSA-N

Formula: C7H16O2

SMILES: CC(C)(O)CC(C)(C)O

Molecular Weight: 132.20

CAS: 24892-49-7



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-259.90	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-509.77	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	7.23	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	61.94	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	0.918		Crippen Method
P_c	3594.25	kPa	Joback Method
T_{boil}	537.46	K	Joback Method
T_c	710.47	K	Joback Method
T_{fus}	295.13	K	Joback Method
V_c	0.444	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	306.05	J/mol×K	537.46	Joback Method
η	0.0000557	Paxs	537.46	Joback Method

Sources

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

NIST Webbook:

[http://webbook.nist.gov/cgi/inchi/InChI=1S/C7H16O2/c1-6\(2,8\)5-7\(3,4\)9/h8-9H,5H2,1-4H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C7H16O2/c1-6(2,8)5-7(3,4)9/h8-9H,5H2,1-4H3)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

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

η : Dynamic viscosity (Paxs).

$\Delta_f G^\circ$: 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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