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
$\Delta_f G°$	-259.90	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-509.77	kJ/mol	Joback Method
$\Delta_{fus} H°$	7.23	kJ/mol	Joback Method
$\Delta_{vap} H°$	61.94	kJ/mol	Joback Method
$logP_{oct/wat}$	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
$C_{p,gas}$	306.05	J/mol×K	537.46	Joback Method
η	0.0000557	Pa×s	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
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).
η: Dynamic viscosity (Pa×s).
$\Delta_f G°$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f H°_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus} H°$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap} H°$: Enthalpy of vaporization at standard conditions (kJ/mol).
***log*P$_{oct/wat}$**: 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^3/kg-mol).