



>>Entry Name: **2,2-Dimethyl-1,3-propanediol**, 9CI, 8CI

Synonym(s): Neopentyl glycol. 2,2-Dimethylolpropane. NPG. Dimethyltrimethylene glycol

CAS Registry Number: 126-30-7

$(\text{H}_3\text{C})_2\text{C}(\text{CH}_2\text{OH})_2$

Molecular Formula:  $\text{C}_5\text{H}_{12}\text{O}_2$

Molecular Weight: 104.149

Accurate Mass: 104.08373

Percentage Composition: C 57.66%; H 11.61%; O 30.72%

Source/Synthesis: Manuf. by aldol addition of isobutyraldehyde to formaldehyde followed by catalytic hydrogenation

Use/Importance: Starting materials for polyesters and polyurethanes. Used in manuf. of coating materials, polymers, hardeners, pharmaceuticals, pesticides, lubricants and plasticizers

Physical Description: Needles ( $\text{C}_6\text{H}_6$ )

Melting Point: Mp 129°

Boiling Point: Bp<sub>747</sub> 206°. Bp<sub>15</sub> 125-130°

Solubility: Part. sol.  $\text{H}_2\text{O}$ ; misc. EtOH,  $\text{Et}_2\text{O}$

Hazard & Toxicity: Fl. p. 129° (oc), autoignition temp. 399°. Low acute tox.

Aldrich: 12658-6

Fluka: 41510

>>Derivative: Di-Ac

CAS Registry Number: 13431-57-7

Molecular Formula:  $\text{C}_9\text{H}_{16}\text{O}_4$

Molecular Weight: 188.223

Accurate Mass: 188.10486

Percentage Composition: C 57.43%; H 8.57%; O 34.00%

Physical Description: Liq.

Boiling Point: Bp 208-209°. Bp<sub>15</sub> 105-108°

>>Derivative: Dibenzoyl

CAS Registry Number: 4196-89-8

Molecular Formula:  $\text{C}_{19}\text{H}_{20}\text{O}_4$

Molecular Weight: 312.365

Accurate Mass: 312.13616

Percentage Composition: C 73.06%; H 6.45%; O 20.49%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 48-49°

Aldrich: 45803-1

>>Derivative: Di-2-propenoyl

CAS Registry Number: 2223-82-7

Molecular Formula:  $\text{C}_{11}\text{H}_{16}\text{O}_4$

Molecular Weight: 212.245

Accurate Mass: 212.10486

Percentage Composition: C 62.25%; H 7.60%; O 30.15%

Use/Importance: Cross-linking monomer

Density:  $d^{20}_4$  1.031

Refractive Index:  $n^{20}_D$  1.4530

Aldrich: 40825-5

>>Derivative: Di-2-methyl-2-propenoyl

CAS Registry Number: 1985-51-9

Molecular Formula:  $\text{C}_{13}\text{H}_{20}\text{O}_4$

Molecular Weight: 240.299

Accurate Mass: 240.13616

Percentage Composition: C 64.98%; H 8.39%; O 26.63%

Use/Importance: Cross-linking monomer

Boiling Point: Bp<sub>0.6</sub> 87°

Density:  $d^{20}_4$  1.003

Refractive Index:  $n^{20}_D$  1.4530

Aldrich: 40824-7