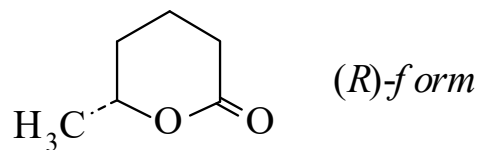




>>Entry Name: Tetrahydro-6-methyl-2*H*-pyran-2-one, 9CI

ENTRY UNDER REVIEW

Synonym(s): 5-Hexanolactone. 5-Caprolactone. 5-Hydroxyhexanoic acid lactone. 5-Hexanolide. 5-Methyl- δ -valerolactone. Dihydrosorbinol. δ -Hexalactone. FEMA 3167



CAS Registry Number: 823-22-3

Molecular Formula: $\text{C}_6\text{H}_{10}\text{O}_2$

Molecular Weight: 114.144

Accurate Mass: 114.06808

Percentage Composition: C 63.14%; H 8.83%; O 28.03%

Biological Source: Isol. from coconut oil (*Cocos nucifera*), heated milk fat, butter, chicken fat and yoghurt. Also formed in var. fruits e.g. papaya, pineapple, raspberry, strawberry and plums. Flavouring ingredient

Aldrich: W31670-9

>>Variant: (*R*)-form

CAS Registry Number: 43112-32-9

Molecular Formula: $\text{C}_6\text{H}_{10}\text{O}_2$

Molecular Weight: 114.144

Accurate Mass: 114.06808

Percentage Composition: C 63.14%; H 8.83%; O 28.03%

Melting Point: Mp 22-24°

Boiling Point: Bp₃ 85-90°

Optical Rotation: $[\alpha]_{\text{D}}^{20} +37.2$ (c, 1.825 in EtOH)

>>Variant: (*S*)-form

CAS Registry Number: 16320-13-1

Molecular Formula: $\text{C}_6\text{H}_{10}\text{O}_2$

Molecular Weight: 114.144

Accurate Mass: 114.06808

Percentage Composition: C 63.14%; H 8.83%; O 28.03%

Melting Point: Mp 31°

Boiling Point: Bp_{11.5} 103-104° (lit. gives a pressure range)

Optical Rotation: $[\alpha]_{\text{D}}^{19} -51$ (EtOH)

Refractive Index: n_{D}^{22} 1.4426

>>Variant: ($\pm$)-form

CAS Registry Number: 26991-67-3

Molecular Formula: $\text{C}_6\text{H}_{10}\text{O}_2$

Molecular Weight: 114.144

Accurate Mass: 114.06808

Percentage Composition: C 63.14%; H 8.83%; O 28.03%

Use/Importance: Flavour ingredient

Physical Description: Needles

Melting Point: Mp 17-19°

Boiling Point: Bp 230-231°. Bp₅ 100-100.5°

Solubility: Misc. H_2O

Other Data: Polymerises on standing

References: