«alpha»-Acetobutyrolactone

Other names: 2(3H)-Furanone, 3-acetyldihydro-
2-Acetyl-4-hydroxybutyric acid «gamma»-lactone
2-Acetyl-«gamma»-butyrolactone
2-Oxo-3-acetyltetrahydrofuran
2-acetylbutyrolactone
3-Acetyl-2(3H)-4,5-dihydrofuranone
3-Acetyltetrahydro-2-furanone
3-acetyldihydrofuran-2(3H)-one
Dihydro-3-acetyl-2(3H)-furanone
NSC 2019
«alpha»-(2-Hydroxyethyl)acetoacetic acid «gamma»-lactone
«alpha»-Acetyl-«gamma»-butyrolactone
«alpha»-Acetyl-«gamma»-hydroxybutyric acid «gamma»-lactone
«alpha»-Acetylbutyrolactone

Inchi: InChI=1S/C6H8O3/c1-4(7)5-2-3-9-6(5)8/h5H,2-3H2,1H3

InchiKey: OMQHDIHZSDEIFH-UHFFFAOYSA-N

Formula: C6H8O3

SMILES: CC(=O)C1CCOC1=O

Mol. weight [g/mol]: 128.13

CAS: 517-23-7

Physical Properties

Property code	Value	Unit	Source
gf	-301.44	kJ/mol	Joback Method
hf	-488.97	kJ/mol	Joback Method
hfus	14.32	kJ/mol	Joback Method
hvap	44.71	kJ/mol	Joback Method
log10ws	-0.13		Crippen Method
logp	0.138		Crippen Method
mcvol	93.550	ml/mol	McGowan Method
pc	4299.92	kPa	Joback Method
rinpol	1108.00		NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1108.00		NIST Webbook
tb	500.60	K	Joback Method
tc	728.46	K	Joback Method
tf	313.00	K	Joback Method

vc	0.346	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.14	J/mol×K	500.60	Joback Method
cpg	221.35	J/mol×K	538.58	Joback Method
cpg	232.98	J/mol×K	576.55	Joback Method
cpg	244.01	J/mol×K	614.53	Joback Method
cpg	254.44	J/mol×K	652.50	Joback Method
cpg	264.24	J/mol×K	690.48	Joback Method
cpg	273.42	J/mol×K	728.46	Joback Method
pvap	60.05	kPa	505.80	Density, Viscosity, and Vapor-Liquid Equilibrium Data for the Binary Mixture at Atmosphere Pressure: Cyclopropyl Methyl Ketone + 2-Acetylbutyrolactone, Cyclopropyl Methyl Ketone + 5-Chloro-2-pentanone
pvap	88.01	kPa	523.30	Density, Viscosity, and Vapor-Liquid Equilibrium Data for the Binary Mixture at Atmosphere Pressure: Cyclopropyl Methyl Ketone + 2-Acetylbutyrolactone, Cyclopropyl Methyl Ketone + 5-Chloro-2-pentanone
pvap	78.10	kPa	517.30	Density, Viscosity, and Vapor-Liquid Equilibrium Data for the Binary Mixture at Atmosphere Pressure: Cyclopropyl Methyl Ketone + 2-Acetylbutyrolactone, Cyclopropyl Methyl Ketone + 5-Chloro-2-pentanone

pvap	69.06	kPa	511.50	Density, Viscosity, and Vapor-Liquid Equilibrium Data for the Binary Mixture at Atmosphere Pressure: Cyclopropyl Methyl Ketone + 2-Acetylbutyrolactone, Cyclopropyl Methyl Ketone + 5-Chloro-2-pentanone
pvap	103.54	kPa	530.80	Density, Viscosity, and Vapor-Liquid Equilibrium Data for the Binary Mixture at Atmosphere Pressure: Cyclopropyl Methyl Ketone + 2-Acetylbutyrolactone, Cyclopropyl Methyl Ketone + 5-Chloro-2-pentanone
pvap	40.17	kPa	489.40	Density, Viscosity, and Vapor-Liquid Equilibrium Data for the Binary Mixture at Atmosphere Pressure: Cyclopropyl Methyl Ketone + 2-Acetylbutyrolactone, Cyclopropyl Methyl Ketone + 5-Chloro-2-pentanone
pvap	30.05	kPa	478.20	Density, Viscosity, and Vapor-Liquid Equilibrium Data for the Binary Mixture at Atmosphere Pressure: Cyclopropyl Methyl Ketone + 2-Acetylbutyrolactone, Cyclopropyl Methyl Ketone + 5-Chloro-2-pentanone

pvap	20.00	kPa	464.50	Density, Viscosity, and Vapor-Liquid Equilibrium Data for the Binary Mixture at Atmosphere Pressure: Cyclopropyl Methyl Ketone + 2-Acetylbutyrolactone, Cyclopropyl Methyl Ketone + 5-Chloro-2-pentanone
pvap	10.00	kPa	445.10	Density, Viscosity, and Vapor-Liquid Equilibrium Data for the Binary Mixture at Atmosphere Pressure: Cyclopropyl Methyl Ketone + 2-Acetylbutyrolactone, Cyclopropyl Methyl Ketone + 5-Chloro-2-pentanone
pvap	6.98	kPa	434.60	Density, Viscosity, and Vapor-Liquid Equilibrium Data for the Binary Mixture at Atmosphere Pressure: Cyclopropyl Methyl Ketone + 2-Acetylbutyrolactone, Cyclopropyl Methyl Ketone + 5-Chloro-2-pentanone
pvap	4.61	kPa	425.50	Density, Viscosity, and Vapor-Liquid Equilibrium Data for the Binary Mixture at Atmosphere Pressure: Cyclopropyl Methyl Ketone + 2-Acetylbutyrolactone, Cyclopropyl Methyl Ketone + 5-Chloro-2-pentanone

pvap	2.92	kPa	415.30	Density, Viscosity, and Vapor-Liquid Equilibrium Data for the Binary Mixture at Atmosphere Pressure: Cyclopropyl Methyl Ketone + 2-Acetylbutyrolactone, Cyclopropyl Methyl Ketone + 5-Chloro-2-pentanone
pvap	1.77	kPa	405.20	Density, Viscosity, and Vapor-Liquid Equilibrium Data for the Binary Mixture at Atmosphere Pressure: Cyclopropyl Methyl Ketone + 2-Acetylbutyrolactone, Cyclopropyl Methyl Ketone + 5-Chloro-2-pentanone
pvap	1.02	kPa	395.10	Density, Viscosity, and Vapor-Liquid Equilibrium Data for the Binary Mixture at Atmosphere Pressure: Cyclopropyl Methyl Ketone + 2-Acetylbutyrolactone, Cyclopropyl Methyl Ketone + 5-Chloro-2-pentanone
pvap	0.55	kPa	385.00	Density, Viscosity, and Vapor-Liquid Equilibrium Data for the Binary Mixture at Atmosphere Pressure: Cyclopropyl Methyl Ketone + 2-Acetylbutyrolactone, Cyclopropyl Methyl Ketone + 5-Chloro-2-pentanone

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	380.70	K	0.70	NIST Webbook
tbrp	404.50 ± 1.50	K	2.40	NIST Webbook
tbrp	404.00 ± 1.00	K	2.40	NIST Webbook

Sources

Density, Viscosity, and Vapor-Liquid Equilibrium Data for the Binary Mixture at Atmospheric Pressure: Cyclopropyl Methyl Ketone + 2-Acetylbutyrolactone, Cyclopropyl Methyl Ketone + 5-Chloro-2-pentanone:	https://www.doi.org/10.1021/acs.jced.7b00344
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C517237&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume