

# Acetoin

<b>Other names:</b>	2-Butanone, 3-hydroxy- «gamma»-Hydroxy-«beta»-oxobutane Acetyl methyl carbinol Dimethylketol Methanol, acetylmethyl- 1-Hydroxyethyl methyl ketone 2-Hydroxy-3-butanone 2,3-Butanolone 3-Hydroxy-2-butanone 2-Butanol-3-one UN 2621 2-Hydroxy-3-oxobutane 3-Hydroxybutan-2-one 3-Hydroxyl-2-butanone Butan-2-one, 3-hydroxy- NSC 7609 acetoine 3-hydroxy-2-butanone (acetoin) 3-hydroxybutan-2-one (acetoin) 3-hydroxy-2-butanone (acetoine) acetoin (3-hydroxy-2-butanone)
<b>Inchi:</b>	InChI=1S/C4H8O2/c1-3(5)4(2)6/h3,5H,1-2H3
<b>InchiKey:</b>	ROWKJAVDOGW PAT-UHFFFAOYSA-N
<b>Formula:</b>	C4H8O2
<b>SMILES:</b>	CC(=O)C(C)O
<b>Mol. weight [g/mol]:</b>	88.11
<b>CAS:</b>	513-86-0

## Physical Properties

Property code	Value	Unit	Source
gf	-285.38	kJ/mol	Joback Method
hf	-395.98	kJ/mol	Joback Method
hfus	8.28	kJ/mol	Joback Method
hvap	48.70 ± 0.40	kJ/mol	NIST Webbook
log10ws	-0.15		Crippen Method
logp	-0.044		Crippen Method

mcvol	74.660	ml/mol	McGowan Method
pc	4829.24	kPa	Joback Method
rinpol	709.00		NIST Webbook
rinpol	661.00		NIST Webbook
rinpol	693.00		NIST Webbook
rinpol	712.00		NIST Webbook
rinpol	714.00		NIST Webbook
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rinpol	666.00		NIST Webbook
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tb	436.53	K	Joback Method
tc	614.26	K	Joback Method
tf	230.59	K	Joback Method
vc	0.279	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	146.25	J/molxK	436.53	Joback Method
cpg	153.06	J/molxK	466.15	Joback Method
cpg	159.59	J/molxK	495.77	Joback Method

cpg	165.85	J/mol×K	525.39	Joback Method
cpg	171.84	J/mol×K	555.02	Joback Method
cpg	177.58	J/mol×K	584.64	Joback Method
cpg	183.06	J/mol×K	614.26	Joback Method
dvisc	0.0663519	Paxs	230.59	Joback Method
dvisc	0.0146308	Paxs	264.91	Joback Method
dvisc	0.0045636	Paxs	299.24	Joback Method
dvisc	0.0018091	Paxs	333.56	Joback Method
dvisc	0.0008524	Paxs	367.88	Joback Method
dvisc	0.0004566	Paxs	402.21	Joback Method
dvisc	0.0002698	Paxs	436.53	Joback Method
hvapt	38.40	kJ/mol	345.50	NIST Webbook

## Sources

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C513860&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C513860&amp;Units=SI</a>
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## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</b>	Non-polar retention indices
<b>ripola:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

**tf:** Normal melting (fusion) point

**vc:** Critical Volume

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