Acetoin

Other names:	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)
	2-Butanone, 3-hydroxy-, (.+/-.)-
Inchi:	InChI=1S/C4H8O2/c1-3(5)4(2)6/h3,5H,1-2H3
InchiKey:	ROWKJAVDOGWPAT-UHFFFAOYSA-N
Formula:	C4H8O2
SMILES:	CC(=O)C(C)O
Mol. weight [g/mol]:	88.11
CAS:	52217-02-4

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	47.53	kJ/mol	Joback Method
log10ws	-0.15		Crippen Method

logp	-0.044		Crippen Method
mcvol	74.660	ml/mol	McGowan Method
pc	4829.24	kPa	Joback Method
tb	416.20	K	NIST Webbook
tc	614.26	K	Joback Method
tf	230.59	K	Joback Method
vc	0.279	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	146.25	J/mol×K	436.53	Joback Method
cpg	153.06	J/mol×K	466.15	Joback Method
cpg	159.59	J/mol×K	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	Pa×s	230.59	Joback Method
dvisc	0.0146308	Pa×s	264.91	Joback Method
dvisc	0.0045636	Pa×s	299.24	Joback Method
dvisc	0.0018091	Pa×s	333.56	Joback Method
dvisc	0.0008524	Pa×s	367.88	Joback Method
dvisc	0.0004566	Pa×s	402.21	Joback Method
dvisc	0.0002698	Pa×s	436.53	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	310.20	K	1.50	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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=C52217024&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume