3-Hydroxy-3-methyl-2-butanone

Other names:	2-Butanone, 3-hydroxy-3-methyl-
	Dimethylacetylcarbinol
	3-Hydroxy-3-methylbutanone
	1-Hydroxy-1-methylethyl methyl ketone
	Methylacetoin
	3-Methylacetoin
	Acetyldimethylcarbinol
	2-Hydroxy-2-methyl-3-butanone
	2-Methyl-2-hydroxybutan-3-one
	3-hydroxy-3-ethylbutanone
Inchi:	InChI=1S/C5H10O2/c1-4(6)5(2,3)7/h7H,1-3H3
InchiKey:	BNDRWEVUODOUDW-UHFFFAOYSA-N
Formula:	C5H10O2
SMILES:	CC(=O)C(C)(C)O
Mol. weight [g/mol]:	102.13
CAS:	115-22-0

Physical Properties

Property code	Value	Unit	Source
gf	-271.68	kJ/mol	Joback Method
hf	-420.09	kJ/mol	Joback Method
hfus	6.98	kJ/mol	Joback Method
hvap	48.85	kJ/mol	Joback Method
log10ws	-0.57		Crippen Method
logp	0.346		Crippen Method
mcvol	88.750	ml/mol	McGowan Method
pc	4305.56	kPa	Joback Method
rinpol	700.00		NIST Webbook
rinpol	778.00		NIST Webbook
rinpol	779.00		NIST Webbook
rinpol	691.00		NIST Webbook
ripol	1246.00		NIST Webbook
ripol	1246.00		NIST Webbook
ripol	1262.00		NIST Webbook
ripol	1262.00		NIST Webbook
ripol	1247.00		NIST Webbook
ripol	1243.00		NIST Webbook

ripol	1262.00		NIST Webbook
ripol	1238.00		NIST Webbook
tb	413.20	K	NIST Webbook
tc	639.96	K	Joback Method
tf	259.28	K	Joback Method
vc	0.330	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.22	J/mol×K	639.96	Joback Method
cpg	225.71	J/mol×K	609.41	Joback Method
cpg	218.81	J/mol×K	578.85	Joback Method
cpg	211.50	J/mol×K	548.29	Joback Method
cpg	203.75	J/mol×K	517.73	Joback Method
cpg	195.55	J/mol×K	487.18	Joback Method
cpg	186.87	J/mol×K	456.62	Joback Method
dvisc	0.0365089	Pa×s	259.28	Joback Method
dvisc	0.0002510	Pa×s	456.62	Joback Method
dvisc	0.0004171	Pa×s	423.73	Joback Method
dvisc	0.0007550	Pa×s	390.84	Joback Method
dvisc	0.0015240	Pa×s	357.95	Joback Method
dvisc	0.0035460	Pa×s	325.06	Joback Method
dvisc	0.0099787	Pa×s	292.17	Joback Method
hvapt	41.10	kJ/mol	368.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C115220&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume