2-Butanone, 3,3-dimethyl-

Other names:	.alpha.,.alpha.,.alpha.-trimethylacetone
	1,1,1-TRIMETHYLACETONE
	1,1-Dimethylethyl methyl ketone
	2,2-Dimethyl-3-butanone
	2,2-Dimethylbutanone
	3,3-DIMETHYL-2-BUTANONE
	3,3-Dimethyl-butan-2-one
	3,3-Dimethylbutanone
	3,3-dimethylbutanone-2
	Ketone, t-butyl methyl
	Ketone, tert-butyl methyl
	Methyl t-butyl ketone
	Methyl tert-butyl ketone
	NSC 935
	PINACOLINE
	Pinacolin
	Pinacolone
	Pinakolin
	t-Butyl methyl ketone
	tert-Butyl methyl ketone
	tert-C4H9COCH3
Inchi:	InChI=1S/C6H12O/c1-5(7)6(2,3)4/h1-4H3
InchiKey:	PJGSXYOJTGTZAV-UHFFFAOYSA-N
Formula:	C6H12O
SMILES:	CC(=O)C(C)(C)C
Mol. weight [g/mol]:	100.16
CAS:	75-97-8

Physical Properties

Property code	Value	Unit	Source
affp	840.10	kJ/mol	NIST Webbook
basg	809.60	kJ/mol	NIST Webbook
basg	808.20	kJ/mol	NIST Webbook
basg	810.00 ± 0.40	kJ/mol	NIST Webbook
chl	-3747.49 ± 0.81	kJ/mol	NIST Webbook
gf	-126.44	kJ/mol	Joback Method

hf	-290.67 ± 0.88	kJ/mol	NIST Webbook
hfl	-328.54 ± 0.28	kJ/mol	NIST Webbook
hfus	5.48	kJ/mol	Joback Method
hvap	37.90 ± 0.10	kJ/mol	NIST Webbook
hvap	38.00	kJ/mol	NIST Webbook
hvap	37.87 ± 0.08	kJ/mol	NIST Webbook
hvap	38.30	kJ/mol	NIST Webbook
ie	9.21	eV	NIST Webbook
ie	9.18 ± 0.03	eV	NIST Webbook
ie	9.17 ± 0.03	eV	NIST Webbook
ie	9.14 ± 0.01	eV	NIST Webbook
ie	8.88 ± 0.04	eV	NIST Webbook
ie	9.24	eV	NIST Webbook
ie	9.11 ± 0.01	eV	NIST Webbook
ie	9.17 ± 0.06	eV	NIST Webbook
ie	9.12 ± 0.01	eV	NIST Webbook
ie	9.40	eV	NIST Webbook
ie	9.14 ± 0.03	eV	NIST Webbook
log10ws	-0.72		Estimated Solubility Method
log10ws	-0.72		Aqueous Solubility Prediction Method
logp	1.621		Crippen Method
mcvol	96.970	ml/mol	McGowan Method
pc	3411.87	kPa	Joback Method
rinpol	690.48		NIST Webbook
rinpol	697.44		NIST Webbook
rinpol	697.00		NIST Webbook
rinpol	692.00		NIST Webbook
rinpol	693.00		NIST Webbook
rinpol	696.00		NIST Webbook
rinpol	698.00		NIST Webbook
rinpol	675.00		NIST Webbook
rinpol	693.30		NIST Webbook
rinpol	672.00		NIST Webbook
rinpol	665.00		NIST Webbook
rinpol	692.00		NIST Webbook
rinpol	692.00		NIST Webbook
rinpol	681.00		NIST Webbook
rinpol	705.00		NIST Webbook
rinpol	665.00		NIST Webbook
rinpol	693.00		NIST Webbook
rinpol	692.00		NIST Webbook
rinpol	695.00		NIST Webbook
rinpol	692.00		NIST Webbook

rinpol	692.00		NIST Webbook
rinpol	693.00		NIST Webbook
rinpol	705.00		NIST Webbook
rinpol	698.00		NIST Webbook
rinpol	665.00		NIST Webbook
rinpol	692.00		NIST Webbook
rinpol	693.10		NIST Webbook
rinpol	695.47		NIST Webbook
rinpol	698.00		NIST Webbook
rinpol	693.10		NIST Webbook
rinpol	691.81		NIST Webbook
rinpol	695.47		NIST Webbook
rinpol	685.00		NIST Webbook
ripol	978.00		NIST Webbook
ripol	949.00		NIST Webbook
ripol	968.50		NIST Webbook
ripol	986.30		NIST Webbook
ripol	968.00		NIST Webbook
ripol	978.00		NIST Webbook
ripol	949.00		NIST Webbook
ripol	978.00		NIST Webbook
ripol	978.00		NIST Webbook
ripol	980.20		NIST Webbook
ripol	974.30		NIST Webbook
ripol	986.30		NIST Webbook
ripol	960.00		NIST Webbook
sl	282.40	J/mol×K	NIST Webbook
tb	379.35 ± 0.50	K	NIST Webbook
tb	378.75 ± 1.00	K	NIST Webbook
tb	378.65 ± 0.50	K	NIST Webbook
tb	379.20 ± 0.50	K	NIST Webbook
tb	379.15 ± 1.50	K	NIST Webbook
tb	379.65 ± 0.30	K	NIST Webbook
tb	378.65 ± 2.00	K	NIST Webbook
tb	378.85 ± 1.00	K	NIST Webbook
tb	376.15 ± 5.00	K	NIST Webbook
tb	379.00 ± 2.50	K	NIST Webbook
tb	447.50 ± 0.30	K	NIST Webbook
tb	377.15 ± 2.00	K	NIST Webbook
tb	378.15 ± 3.00	K	NIST Webbook
tb	379.40 ± 1.00	K	NIST Webbook
tb	377.65 ± 1.00	K	NIST Webbook
tb	378.95 ± 1.00	K	NIST Webbook
tb	379.30 ± 1.00	K	NIST Webbook

tb	378.15 ± 1.00	K	NIST Webbook
tb	379.15 ± 0.50	K	NIST Webbook
tb	378.15 ± 1.00	K	NIST Webbook
tb	378.15 ± 1.00	K	NIST Webbook
tb	378.15 ± 2.00	K	NIST Webbook
tb	379.20	K	NIST Webbook
tb	378.15 ± 1.00	K	NIST Webbook
tb	378.90 ± 0.50	K	NIST Webbook
tb	383.40 ± 5.00	K	NIST Webbook
tb	399.15 ± 0.50	K	NIST Webbook
tb	363.15	K	NIST Webbook
tb	377.00 ± 2.00	K	NIST Webbook
tb	378.65 ± 0.50	K	NIST Webbook
tb	378.35 ± 0.50	K	NIST Webbook
tb	379.00 ± 0.30	K	NIST Webbook
tb	379.40 ± 0.50	K	NIST Webbook
tb	379.20 ± 0.50	K	NIST Webbook
tb	379.65 ± 0.50	K	NIST Webbook
tb	379.35 ± 0.50	K	NIST Webbook
tb	378.63 ± 0.20	K	NIST Webbook
tb	379.30	K	NIST Webbook
tc	562.90	K	NIST Webbook
tf	223.40 ± 2.00	K	NIST Webbook
tf	220.65	K	Aqueous Solubility Prediction Method
tf	220.65 ± 0.50	K	NIST Webbook
tf	220.65 ± 0.50	K	NIST Webbook
tt	221.74 ± 0.05	K	NIST Webbook
vc	0.366	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	182.00 ± 0.27	J/mol×K	385.67	NIST Webbook
cpg	185.98 ± 0.28	J/mol×K	399.53	NIST Webbook
cpg	187.61 ± 0.28	J/mol×K	405.07	NIST Webbook
cpg	189.16 ± 0.28	J/mol×K	410.70	NIST Webbook
cpg	183.97 ± 0.28	J/mol×K	392.13	NIST Webbook
cpl	206.90	J/mol×K	298.15	NIST Webbook
cpl	207.30	J/mol×K	298.15	NIST Webbook
dvisc	0.0009573	Pa×s	298.52	Joback Method

dvisc	0.0015819	Pa×s	268.93	Joback Method
dvisc	0.0004499	Pa×s	357.72	Joback Method
dvisc	0.0066076	Pa×s	209.73	Joback Method
dvisc	0.0006343	Pa×s	328.12	Joback Method
dvisc	0.0003363	Pa×s	387.32	Joback Method
dvisc	0.0029595	Pa×s	239.33	Joback Method
hfust	11.33	kJ/mol	221.74	NIST Webbook
hfust	11.34	kJ/mol	221.70	NIST Webbook
hfust	11.34	kJ/mol	221.70	NIST Webbook
hvapt	50.78	kJ/mol	441.40	NIST Webbook
hvapt	33.39	kJ/mol	379.30	NIST Webbook
hvapt	36.10	kJ/mol	338.00	NIST Webbook
hvapt	38.30	kJ/mol	345.50	NIST Webbook
hvapt	33.10	kJ/mol	529.00	NIST Webbook
hvapt	33.80	kJ/mol	452.50	NIST Webbook
hvapt	34.90	kJ/mol	381.50	NIST Webbook
hvapt	36.90	kJ/mol	346.00	NIST Webbook
hvapt	35.00 ± 0.10	kJ/mol	348.00	NIST Webbook
hvapt	35.40 ± 0.10	kJ/mol	343.00	NIST Webbook
hvapt	35.80 ± 0.10	kJ/mol	338.00	NIST Webbook
hvapt	36.70 ± 0.10	kJ/mol	328.00	NIST Webbook
hvapt	36.90 ± 0.10	kJ/mol	323.00	NIST Webbook
hvapt	37.50 ± 0.10	kJ/mol	313.00	NIST Webbook
hvapt	37.80 ± 0.10	kJ/mol	308.00	NIST Webbook
sfust	51.10	J/mol×K	221.74	NIST Webbook
sfust	51.04	J/mol×K	221.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.59883e+01
Coeff. B	-3.80943e+03
Coeff. C	-5.07410e+01
Temperature range (K), min.	293.37
Temperature range (K), max.	407.54

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.43512e+01
Coeff. B	-6.93657e+03
Coeff. C	-8.79890e+00
Coeff. D	5.59014e-06
Temperature range (K), min.	277.15
Temperature range (K), max.	405.00

Sources

Phase Equilibrium on Extraction Methylphenols from Aqueous Solution with3,3-Dimethyl-2-butanone at 333.2 K and 353.2 K:	https://www.doi.org/10.1021/acs.jced.7b00932
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Screening solvents to extract phenol from aqueous solutions by the COSMO-SAC model and extraction process simulation:	https://www.doi.org/10.1016/j.fluid.2017.08.007
Air-Water Partitioning of C5 and C6 Alkanones: Measurement, Critical Comparison, Correlation, and Prediction:	https://www.doi.org/10.1021/acs.jced.9b00726
Isothermal vapor-liquid equilibria in the binary and ternary systems composed of tert-butyl methyl ether, 3,3-dimethyl-2-butanone and 2,2-dimethyl-1-propanol:	https://www.doi.org/10.1016/j.fluid.2009.01.016
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1201.mol
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75978&Units=SI
Liquid Liquid Phase Equilibria for the Ternary Water + Acetic Acid + 3,3-Dimethyl-2-butanone System at (298.15, 313.15 and 323.15) K:	https://www.doi.org/10.1021/acs.jced.5b00370
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1201
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Liquid Phase Equilibria of the Water + Propionic or Butyric Acid + Methyl tert-Butylketone Ternary Systems at (298.15 and 323.15) K:	https://www.doi.org/10.1021/acs.jced.5b00214
Liquid–Liquid Equilibrium for the Ternary Systems Methyl tert-Butyl Ketone + 1-Hexanol + Water at (293.2, 313.2, and 323.2) K:	https://www.doi.org/10.1021/acs.jced.6b00825
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions

hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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