3-Penten-2-one, 4-methyl-

Other names:	(CH3)2C=CHC(=O)CH3
	2,2-Dimethylvinyl methyl ketone
	2-Methyl-2-penten-4-one
	2-Methyl-2-pentenone-4
	2-Methyl-4-oxo-2-pentene
	2-Methylpent-2-en-4-one
	3-Isohexen-2-one
	4-METHYL-3-PENTEN-2-ONE
	4-Methyl-3-penten-2-on
	4-Methyl-3-pentene-2-one
	4-Methylpent-3-en-2-one
	4-Metil-3-penten-2-one
	4-methyl-3-penten-2-one (mesityl oxide)
	Acetone, isopropylidene-
	ISOBUTENYL METHYL KETONE
	ISOPROPYLIDENEACETONE
	MIBK
	Mesityl oxide
	Mesityloxid
	Mesityloxyde
	Methyl 2,2-dimethylvinyl ketone
	Methyl 2-methyl-1-propenyl ketone
	Methyl isobutenyl ketone
	NSC 38717
	Ossido di mesitile
	Oxyde de mesityle
	UN 1229
Inchi:	InChI=1S/C6H10O/c1-5(2)4-6(3)7/h4H,1-3H3
InchiKey:	SHOJXDKTYKFBRD-UHFFFAOYSA-N
Formula:	C6H10O
SMILES:	CC(=O)C=C(C)C
Mol. weight [g/mol]:	98.14
CAS:	141-79-7

Physical Properties

Property code	Value	Unit	Source

affp	878.70	kJ/mol	NIST Webbook
basg	846.90	kJ/mol	NIST Webbook
chl	-3540.00	kJ/mol	NIST Webbook
chl	-3569.23 ± 0.48	kJ/mol	NIST Webbook
chl	-3571.00 ± 0.80	kJ/mol	NIST Webbook
chl	-3549.00	kJ/mol	NIST Webbook
gf	-57.61	kJ/mol	Joback Method
hf	-184.50 ± 2.50	kJ/mol	NIST Webbook
hf	-178.28 ± 0.64	kJ/mol	NIST Webbook
hfl	-219.00 ± 0.80	kJ/mol	NIST Webbook
hfl	-220.98 ± 0.58	kJ/mol	NIST Webbook
hfus	11.79	kJ/mol	Joback Method
hvap	42.70 ± 0.30	kJ/mol	NIST Webbook
hvap	42.70 ± 0.28	kJ/mol	NIST Webbook
hvap	44.80	kJ/mol	NIST Webbook
hvap	43.30	kJ/mol	NIST Webbook
ie	9.11	eV	NIST Webbook
ie	9.10 ± 0.02	eV	NIST Webbook
ie	9.08 ± 0.03	eV	NIST Webbook
ie	8.89 ± 0.05	eV	NIST Webbook
log10ws	-1.47		Crippen Method
logp	1.542		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=3)		KDB
pc	4000.00 ± 150.00	kPa	NIST Webbook
rhoc	277.74 ± 9.81	kg/m3	NIST Webbook
rinpol	783.00		NIST Webbook
rinpol	804.00		NIST Webbook
rinpol	798.00		NIST Webbook
rinpol	787.00		NIST Webbook
rinpol	798.00		NIST Webbook
rinpol	797.00		NIST Webbook
rinpol	780.00		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	804.00		NIST Webbook
rinpol	778.00		NIST Webbook
rinpol	782.00		NIST Webbook
rinpol	783.00		NIST Webbook
rinpol	798.00		NIST Webbook
rinpol	798.00		NIST Webbook
rinpol	802.00		NIST Webbook
rinpol	792.00		NIST Webbook
rinpol	778.00		NIST Webbook

rinpol	801.10		NIST Webbook
rinpol	798.00		NIST Webbook
rinpol	792.00		NIST Webbook
rinpol	778.00		NIST Webbook
rinpol	782.00		NIST Webbook
rinpol	771.00		NIST Webbook
rinpol	798.00		NIST Webbook
rinpol	804.00		NIST Webbook
rinpol	798.00		NIST Webbook
ripol	1127.00		NIST Webbook
ripol	1118.00		NIST Webbook
ripol	1118.00		NIST Webbook
ripol	1159.00		NIST Webbook
ripol	1131.00		NIST Webbook
ripol	1136.00		NIST Webbook
ripol	1125.00		NIST Webbook
ripol	1152.00		NIST Webbook
ripol	1129.00		NIST Webbook
ripol	1113.00		NIST Webbook
ripol	1110.00		NIST Webbook
ripol	1140.00		NIST Webbook
ripol	1110.00		NIST Webbook
ripol	1114.00		NIST Webbook
ripol	1118.00		NIST Webbook
ripol	1125.00		NIST Webbook
ripol	1110.00		NIST Webbook
ripol	1137.00		NIST Webbook
ripol	1125.00		NIST Webbook
ripol	1128.00		NIST Webbook
ripol	1127.00		NIST Webbook
ripol	1111.00		NIST Webbook
ripol	1131.00		NIST Webbook
ripol	1140.00		NIST Webbook
ripol	1127.00		NIST Webbook
ripol	1114.00		NIST Webbook
tb	403.15 ± 1.00	K	NIST Webbook
tb	401.54 ± 0.30	K	NIST Webbook
tb	402.60 ± 0.50	K	NIST Webbook
tb	402.90	K	NIST Webbook
tb	402.95	K	NIST Webbook
tb	402.05 ± 1.00	K	NIST Webbook
tb	403.15 ± 1.50	K	NIST Webbook
tb	401.40 ± 1.50	K	NIST Webbook
tb	402.60 ± 0.50	K	NIST Webbook

tc	605.00 ± 2.00	K	NIST Webbook
tf	220.30 ± 0.30	K	NIST Webbook
tf	226.75	K	NIST Webbook
vc	0.358	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	162.72	J/mol×K	394.59	Joback Method
cpg	172.66	J/mol×K	426.37	Joback Method
cpg	182.11	J/mol×K	458.14	Joback Method
cpg	191.09	J/mol×K	489.92	Joback Method
cpg	199.62	J/mol×K	521.70	Joback Method
cpg	207.73	J/mol×K	553.47	Joback Method
cpg	215.42	J/mol×K	585.25	Joback Method
hfust	12.10	kJ/mol	229.60	NIST Webbook
hvapt	41.40 ± 0.30	kJ/mol	372.50	NIST Webbook
hvapt	39.10 ± 0.30	kJ/mol	372.50	NIST Webbook
hvapt	36.50 ± 0.30	kJ/mol	372.50	NIST Webbook
hvapt	33.50 ± 0.60	kJ/mol	372.50	NIST Webbook
hvapt	37.80	kJ/mol	435.00	NIST Webbook
hvapt	41.50	kJ/mol	359.00	NIST Webbook
hvapt	35.20	kJ/mol	401.00	NIST Webbook
rhol	857.60	kg/m3	298.15	Determination and Correlation of Liquid-Liquid Equilibria Data for Water + Cyclohexanol + (Mesityl Oxide, Toluene, and p-Xylene) Ternary Systems at Different Temperatures

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43990e+01

Coeff. B	-3.41585e+03
Coeff. C	-5.34050e+01
Temperature range (K), min.	295.47
Temperature range (K), max.	429.29

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.11275e+01
Coeff. B	-6.98731e+03
Coeff. C	-6.58940e+00
Coeff. D	2.18991e-06
Temperature range (K), min.	220.15
Temperature range (K), max.	600.00

Sources

Measurement and Correlation of Ternary (Liquid + Liquid) Equilibria for Separation of Cyclohexanone from Water via Isophorone or Mesityl Oxide:	https://www.doi.org/10.1021/acs.jced.7b00787
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1225
Liquid-Liquid Equilibria for the Ternary System Mesityl Oxide + Phenol + Water at 298.15, 313.15, and 323.15 K:	https://www.doi.org/10.1021/acs.jced.6b00186
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1225.mol
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Determination and Correlation of Liquid-Liquid Equilibria Data for Water + Cyclohexanol + (Mesityl Oxide, Toluene, and p-Xylene) Ternary Systems at Different Temperatures:	https://www.doi.org/10.1021/acs.jced.7b00674
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C141797&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Liquid phase equilibrium of the ternary systems, water + propionic or butyric acid + mesityl oxide, at (298.2 and 323.2) K:	https://www.doi.org/10.1016/j.jct.2017.03.018
Measurement, correlation and COSMO-SAC prediction of liquid-liquid equilibrium for the ternary systems, mesityl oxide + o-, m-, p-cresol + water, at 333.2 K and 353.2 K:	https://www.doi.org/10.1016/j.fluid.2017.03.002
Modified Wilson Model:	http://link.springer.com/article/10.1007/BF02311772
Liquid-Liquid Equilibrium for Ternary Systems of 2-Pentanone/Mesityl Oxide + Catechol + Water at 298.2, 318.2, and 338.2 K:	https://www.doi.org/10.1021/acs.jced.8b00380
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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

Legend

affp: Proton affinity

basg: Gas basicity

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rhoc:	Critical density
rhol:	Liquid Density
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