4-Heptanone, 2,6-dimethyl-

Other names:	(iso-C4H9)2CO
	2,6-Dimethyl-4-heptanone
	2,6-Dimethyl-heptan-4-on
	2,6-Dimethylheptan-4-one
	2,6-Dimetil-eptan-4-one
	2,6-dimethyl-4-heptanone (diisobutyl ketone)
	DIBK
	Di-isobutylcetone
	Diisobutilchetone
	Diisobutyl ketone
	Diisobutylketon
	ISOVALERONE
	Isobutyl ketone
	NSC 15136
	S-DIISOPROPYLACETONE
	UN 1157
	Valerone
	sym-Diisopropylacetone
Inchi:	InChI=1S/C9H18O/c1-7(2)5-9(10)6-8(3)4/h7-8H,5-6H2,1-4H3
InchiKey:	PTTPXKJBFFKCEK-UHFFFAOYSA-N
Formula:	C9H18O
SMILES:	CC(C)CC(=O)CC(C)C
Mol. weight [g/mol]:	142.24
CAS:	108-83-8

Physical Properties

Property code	Value	Unit	Source
chl	-5705.50 ± 1.10	kJ/mol	NIST Webbook
gf	-108.90	kJ/mol	Joback Method
hf	-357.70 ± 1.20	kJ/mol	NIST Webbook
hfl	-408.60 ± 1.20	kJ/mol	NIST Webbook
hfus	13.62	kJ/mol	Joback Method
hvap	51.00	kJ/mol	NIST Webbook
hvap	50.92 ± 0.04	kJ/mol	NIST Webbook
hvap	50.90 ± 0.10	kJ/mol	NIST Webbook
ie	9.04 ± 0.03	eV	NIST Webbook
ie	8.98 ± 0.01	eV	NIST Webbook

ie	9.01 ± 0.03	eV	NIST Webbook
log10ws	-2.39		Crippen Method
logp	2.648		Crippen Method
mcvol	139.240	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
nfpah	%!d(float64=1)		KDB
pc	2492.52	kPa	Joback Method
rinpol	935.00		NIST Webbook
rinpol	953.00		NIST Webbook
rinpol	955.00		NIST Webbook
rinpol	961.00		NIST Webbook
rinpol	951.20		NIST Webbook
rinpol	962.10		NIST Webbook
rinpol	943.00		NIST Webbook
rinpol	956.00		NIST Webbook
rinpol	983.00		NIST Webbook
rinpol	954.70		NIST Webbook
rinpol	999.00		NIST Webbook
rinpol	956.00		NIST Webbook
rinpol	961.00		NIST Webbook
rinpol	954.70		NIST Webbook
rinpol	953.00		NIST Webbook
rinpol	962.10		NIST Webbook
rinpol	945.00		NIST Webbook
rinpol	955.00		NIST Webbook
ripol	1207.00		NIST Webbook
ripol	1162.00		NIST Webbook
ripol	1207.00		NIST Webbook
ripol	1189.50		NIST Webbook
ripol	1178.00		NIST Webbook
ripol	1207.00		NIST Webbook
tb	438.90 ± 5.00	K	NIST Webbook
tb	441.39 ± 0.10	K	NIST Webbook
tb	441.20 ± 0.60	K	NIST Webbook
tb	441.20 ± 2.00	K	NIST Webbook
tb	442.00 ± 8.00	K	NIST Webbook
tb	442.50 ± 0.80	K	NIST Webbook
tb	442.50 ± 0.60	K	NIST Webbook
tb	397.15 ± 1.00	K	NIST Webbook
tb	442.55	K	NIST Webbook
tb	442.60	K	NIST Webbook
tb	438.15 ± 1.50	K	NIST Webbook
tb	441.00 ± 3.00	K	NIST Webbook
tb	439.00 ± 6.00	K	NIST Webbook

tb	438.15 ± 2.00	K	NIST Webbook
tb	441.30 ± 1.50	K	NIST Webbook
tb	438.00 ± 5.00	K	NIST Webbook
tb	442.50 ± 1.00	K	NIST Webbook
tc	640.10	K	Joback Method
tf	231.60 ± 3.00	K	NIST Webbook
tf	227.00 ± 0.60	K	NIST Webbook
tf	231.70 ± 2.00	K	NIST Webbook
tf	227.11 ± 0.07	K	NIST Webbook
tf	227.00 ± 0.60	K	NIST Webbook
tf	231.65	K	NIST Webbook
vc	0.533	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.81	J/mol×K	640.10	Joback Method
cpg	363.40	J/mol×K	609.80	Joback Method
cpg	297.92	J/mol×K	458.31	Joback Method
cpg	312.19	J/mol×K	488.61	Joback Method
cpg	325.86	J/mol×K	518.91	Joback Method
cpg	338.94	J/mol×K	549.20	Joback Method
cpg	351.45	J/mol×K	579.50	Joback Method
cpl	297.30	J/mol×K	298.15	NIST Webbook
dvisc	0.0003537	Pa×s	417.11	Joback Method
dvisc	0.0002572	Pa×s	458.31	Joback Method
dvisc	0.0112700	Pa×s	211.12	Joback Method
dvisc	0.0035885	Pa×s	252.32	Joback Method
dvisc	0.0015755	Pa×s	293.52	Joback Method
dvisc	0.0008471	Pa×s	334.72	Joback Method
dvisc	0.0005218	Pa×s	375.91	Joback Method
hvapt	45.20 ± 0.10	kJ/mol	358.00	NIST Webbook
hvapt	46.80	kJ/mol	393.50	NIST Webbook
hvapt	38.60	kJ/mol	379.30	NIST Webbook
hvapt	49.80 ± 0.10	kJ/mol	308.00	NIST Webbook
hvapt	49.30 ± 0.10	kJ/mol	313.00	NIST Webbook
hvapt	48.40 ± 0.10	kJ/mol	323.00	NIST Webbook
hvapt	47.90 ± 0.10	kJ/mol	328.00	NIST Webbook
hvapt	47.10 ± 0.10	kJ/mol	338.00	NIST Webbook
hvapt	46.60 ± 0.10	kJ/mol	343.00	NIST Webbook
hvapt	46.10 ± 0.10	kJ/mol	348.00	NIST Webbook

rfi	1.41550		293.15	(Liquid + liquid) equilibria of (water + propionic acid + methyl isoamyl ketone or diisobutyl ketone or ethyl isoamyl keton) at T = 298.2 K
rhol	792.50	kg/m3	313.20	Liquid-liquid equilibrium data and thermophysical properties for ternary systems composed of water, acetic acid and different solvents
rhol	809.04	kg/m3	293.20	Liquid-liquid equilibrium data and thermophysical properties for ternary systems composed of water, acetic acid and different solvents

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50856e+01
Coeff. B	-3.94760e+03
Coeff. C	-6.38620e+01
Temperature range (K), min.	330.63
Temperature range (K), max.	467.75

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.12806e+02
Coeff. B	-9.95574e+03
Coeff. C	-1.43270e+01
Coeff. D	8.33011e-06

Temperature range (K), min.	227.17
Temperature range (K), max.	615.00

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1213.mol
Quaternary phase equilibrium of water-carboxylic acid mixture (formic-propionic acid or acetic-propionic acid)-solvent liquid systems at 298.15 K:	https://www.doi.org/10.1016/j.fluid.2011.09.014
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1213
Extraction of Citric Acid and Maleic Acid from Their Aqueous Solutions Using a Phosphorus-Bonded Extractant: Trioctylphosphine Oxide and a Secondary Amine, Dioctylamine:	https://www.doi.org/10.1021/acs.jced.7b00562
(Liquid + liquid) equilibria of (water + propionic acid + methyl isobutyl ketone (MIBK)) ternary system at T = (293.15 and 298.15) K:	https://www.doi.org/10.1016/j.fluid.2006.10.004
Comparison of Extractability of Oxalic, Citric, Tartaric, and Malic Acid from Dilute Aqueous Solutions Using Dioctylamine and Trioctylphosphine Oxide:	https://www.doi.org/10.1021/acs.jced.8b01155
(Liquid + liquid) equilibrium data and thermophysical properties for ternary systems composed of water, acetic acid and different solvents:	https://www.doi.org/10.1016/j.fluid.2018.10.021
NIST WebBook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C108838&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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
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
rfi:	Refractive Index
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