

5-Hepten-2-one, 6-methyl-

Other names:	2-Methyl-2-hepten-6-one 2-methyl-6-heptenone 2-methylhept-2-en-6-one 5-heptene-2-one, 6-methyl- 6-Methyl hept-5-en-2-one 6-Methyl hept-5-ene-2-one 6-Methyl-5-hepten-2-one 6-Methyl-5-heptene-2-one 6-methyl-5-hepten-2-one Methyl heptenone NSC 15294 Sulcatone methyl-5-hepten-2-one
Inchi:	InChI=1S/C8H14O/c1-7(2)5-4-6-8(3)9/h5H,4,6H2,1-3H3
InchiKey:	UHEPJGULSIKKTU-UHFFFAOYSA-N
Formula:	C8H14O
SMILES:	CC(=O)CCC=C(C)C
Mol. weight [g/mol]:	126.20
CAS:	110-93-0

Physical Properties

Property code	Value	Unit	Source
chl	-4837.80 ± 1.60	kJ/mol	NIST Webbook
gf	-40.77	kJ/mol	Joback Method
hf	-303.70 ± 1.60	kJ/mol	NIST Webbook
hfus	16.97	kJ/mol	Joback Method
hvap	40.19	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.322		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	2871.95	kPa	Joback Method
rinpol	964.00		NIST Webbook
rinpol	963.90		NIST Webbook
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ripol	1338.00	NIST Webbook
ripol	1346.00	NIST Webbook
ripol	1345.00	NIST Webbook
ripol	1328.00	NIST Webbook
ripol	1328.00	NIST Webbook
ripol	1340.00	NIST Webbook
ripol	1327.00	NIST Webbook
ripol	1333.00	NIST Webbook
ripol	1333.00	NIST Webbook
ripol	1314.00	NIST Webbook
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ripol	1341.00		NIST Webbook
ripol	1344.00		NIST Webbook
ripol	1333.00		NIST Webbook
ripol	1336.00		NIST Webbook
ripol	1317.00		NIST Webbook
ripol	1347.00		NIST Webbook
ripol	1321.00		NIST Webbook
ripol	1329.00		NIST Webbook
ripol	1315.00		NIST Webbook
ripol	1334.00		NIST Webbook
tb	446.40 ± 0.50	K	NIST Webbook
tb	446.40 ± 0.50	K	NIST Webbook
tc	627.87	K	Joback Method
tf	210.81	K	Joback Method
vc	0.470	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.78	J/mol×K	565.36	Joback Method
cpg	275.09	J/mol×K	534.11	Joback Method
cpg	263.86	J/mol×K	502.86	Joback Method
cpg	252.05	J/mol×K	471.60	Joback Method
cpg	305.60	J/mol×K	627.87	Joback Method
cpg	295.94	J/mol×K	596.61	Joback Method
cpg	239.66	J/mol×K	440.35	Joback Method
cpl	267.90	J/mol×K	298.35	NIST Webbook
cpl	268.80	J/mol×K	298.35	NIST Webbook
hvapt	44.70 ± 0.20	kJ/mol	389.50	NIST Webbook
hvapt	45.90	kJ/mol	378.50	NIST Webbook
pvap	0.05	kPa	283.86	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation

pvap	0.08	kPa	288.57	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.05	kPa	283.92	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.08	kPa	288.61	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.11	kPa	293.47	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.16	kPa	298.28	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.23	kPa	303.12	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.31	kPa	307.99	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.43	kPa	312.88	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.58	kPa	317.72	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation

pvap	0.77	kPa	322.52	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	1.01	kPa	327.32	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.89	kPa	324.89	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.67	kPa	320.07	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.50	kPa	315.23	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.37	kPa	310.36	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.27	kPa	305.48	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.19	kPa	300.65	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation

pvap	0.14	kPa	295.85	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.10	kPa	291.00	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.07	kPa	286.23	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.05	kPa	283.85	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.08	kPa	288.69	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.11	kPa	293.49	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.16	kPa	298.31	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.23	kPa	303.15	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.31	kPa	308.02	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation

pvap	0.43	kPa	312.90	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.58	kPa	317.75	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.77	kPa	322.56	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	1.02	kPa	327.36	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.89	kPa	324.93	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.67	kPa	320.13	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.50	kPa	315.28	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.37	kPa	310.42	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation

pvap	0.27	kPa	305.54	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.19	kPa	300.69	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.14	kPa	295.88	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.10	kPa	291.02	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.07	kPa	286.24	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.05	kPa	283.86	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.08	kPa	288.59	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.07	kPa	286.18	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.09	kPa	290.97	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation

pvap	0.14	kPa	295.81	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.19	kPa	300.61	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.27	kPa	305.45	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.36	kPa	310.30	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.49	kPa	315.16	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.67	kPa	320.01	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.88	kPa	324.84	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	1.01	kPa	327.28	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation

pvap	0.77	kPa	322.50	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
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Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	346.20	K	2.40	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.27910e+01
Coeff. B	-3.26990e+03
Coeff. C	-6.24000e+01
Temperature range (K), min.	323.92
Temperature range (K), max.	499.58

Sources

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/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation:	https://www.doi.org/10.1016/j.fluid.2014.11.026
Joback Method:	https://www.doi.org/10.1021/acs.jced.8b00126
McGowan Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://link.springer.com/article/10.1007/BF02311772 http://webbook.nist.gov/cgi/cbook.cgi?ID=C110930&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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