3-Heptanone, 6-methyl-

Other names:	2-Methyl-5-heptanone
	6-Methyl-3-heptanone
	6-Methylheptan-3-one
	Ethyl isoamyl ketone
Inchi:	InChI=1S/C8H16O/c1-4-8(9)6-5-7(2)3/h7H,4-6H2,1-3H3
InchiKey:	CCCIYAQYQZQDIZ-UHFFFAOYSA-N
Formula:	C8H16O
SMILES:	CCC(=O)CCC(C)C
Mol. weight [g/mol]:	128.21
CAS:	624-42-0

Physical Properties

Property code	Value	Unit	Source
gf	-114.88	kJ/mol	Joback Method
hf	-326.31	kJ/mol	Joback Method
hfus	14.55	kJ/mol	Joback Method
hvap	39.76	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.402		Crippen Method
mcvol	125.150	ml/mol	McGowan Method
pc	2726.86	kPa	Joback Method
rinpol	941.00		NIST Webbook
ripol	1263.00		NIST Webbook
ripol	1231.00		NIST Webbook
tb	435.87	K	Joback Method
tc	615.20	K	Joback Method
tf	214.85	K	Joback Method
vc	0.483	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.12	J/mol×K	615.20	Joback Method
cpg	314.75	J/mol×K	585.31	Joback Method

cpg	303.91	J/mol×K	555.42	Joback Method
cpg	292.58	J/mol×K	525.54	Joback Method
cpg	280.75	J/mol×K	495.65	Joback Method
cpg	268.41	J/mol×K	465.76	Joback Method
cpg	255.56	J/mol×K	435.87	Joback Method
dvisc	0.0067893	Pa×s	214.85	Joback Method
dvisc	0.0002821	Pa×s	435.87	Joback Method
dvisc	0.0003753	Pa×s	399.03	Joback Method
dvisc	0.0005291	Pa×s	362.20	Joback Method
dvisc	0.0008063	Pa×s	325.36	Joback Method
dvisc	0.0013683	Pa×s	288.52	Joback Method
dvisc	0.0027108	Pa×s	251.69	Joback Method
rfi	1.41940		293.15	(Liquid + liquid) equilibria of (water + propionic acid + methyl isoamyl ketone or diisobutyl ketone or ethyl isoamyl keton) at T = 298.2 K

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51673e+01
Coeff. B	-3.93631e+03
Coeff. C	-6.26780e+01
Temperature range (K), min.	327.22
Temperature range (K), max.	462.07

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

(Liquid + liquid) equilibria of (water + propionic acid + methyl isoamyl ketone or diisobutyl ketone or ethyl isoamyl keton) at T = 298.2 K: https://www.doi.org/10.1016/j.fluid.2006.10.004

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C624420&Units=SI

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

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
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