4-Heptanone, 3-methyl-

Other names: 3-Methyl-4-heptanone
3-methylheptan-4-one
Inchi: InChI=1S/C8H16O/c1-4-6-8(9)7(3)5-2/h7H,4-6H2,1-3H3
InchiKey: NHIMSNHOEAVUKE-UHFFFAOYSA-N
Formula: C8H16O
SMILES: CCCC(=O)C(C)CC
Mol. weight [g/mol]: 128.21
CAS: 15726-15-5

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	923.00		NIST Webbook
rinpol	932.00		NIST Webbook
rinpol	932.00		NIST Webbook
ripol	1403.00		NIST Webbook
ripol	1403.00		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	255.56	J/mol×K	435.87	Joback Method
cpg	268.41	J/mol×K	465.76	Joback Method

cpg	280.75	J/mol×K	495.65	Joback Method
cpg	292.58	J/mol×K	525.54	Joback Method
cpg	303.91	J/mol×K	555.42	Joback Method
cpg	314.75	J/mol×K	585.31	Joback Method
cpg	325.12	J/mol×K	615.20	Joback Method
dvisc	0.0067893	Pa×s	214.85	Joback Method
dvisc	0.0027108	Pa×s	251.69	Joback Method
dvisc	0.0013683	Pa×s	288.52	Joback Method
dvisc	0.0008063	Pa×s	325.36	Joback Method
dvisc	0.0005291	Pa×s	362.20	Joback Method
dvisc	0.0003753	Pa×s	399.03	Joback Method
dvisc	0.0002821	Pa×s	435.87	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47567e+01
Coeff. B	-3.79520e+03
Coeff. C	-6.14820e+01
Temperature range (K), min.	323.78
Temperature range (K), max.	463.30

Sources

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=C15726155&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

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

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
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