

3-Heptanone, 4-methyl-

Other names:	4-Methyl-3-heptanone 4-methyl-3-heptenone
Inchi:	InChI=1S/C8H16O/c1-4-6-7(3)8(9)5-2/h7H,4-6H2,1-3H3
InchiKey:	MVLRILUUXLBENA-UHFFFAOYSA-N
Formula:	C8H16O
SMILES:	CCCC(C)C(=O)CC
Mol. weight [g/mol]:	128.21
CAS:	6137-11-7

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
tb	435.87	K	Joback Method
tc	615.20	K	Joback Method
tf	214.85	K	Joback Method
vc	0.483	m ³ /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	Paxs	214.85	Joback Method
dvisc	0.0027108	Paxs	251.69	Joback Method
dvisc	0.0013683	Paxs	288.52	Joback Method
dvisc	0.0008063	Paxs	325.36	Joback Method
dvisc	0.0005291	Paxs	362.20	Joback Method
dvisc	0.0003753	Paxs	399.03	Joback Method
dvisc	0.0002821	Paxs	435.87	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.48402e+01
Coeff. B	-3.82591e+03
Coeff. C	-6.15380e+01
Temperature range (K), min.	324.44
Temperature range (K), max.	463.05

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=C6137117&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/ci9903071
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

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
p_{vap}:	Vapor pressure
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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