

2-Heptanone, 3-methyl-

Other names:	3-Methyl-2-heptanone 3-Methylheptan-2-one
Inchi:	InChI=1S/C8H16O/c1-4-5-6-7(2)8(3)9/h7H,4-6H2,1-3H3
InchiKey:	UHRZLJZZZDOHEX-UHFFFAOYSA-N
Formula:	C8H16O
SMILES:	CCCCC(C)C(C)=O
Mol. weight [g/mol]:	128.21
CAS:	2371-19-9

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	883.00		NIST Webbook
rinpol	883.00		NIST Webbook
rinpol	883.00		NIST Webbook
rinpol	930.00		NIST Webbook
tb	431.00 ± 8.00	K	NIST Webbook
tb	435.00 ± 3.00	K	NIST Webbook
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	314.75	J/mol×K	585.31	Joback Method

cpg	303.91	J/molxK	555.42	Joback Method
cpg	292.58	J/molxK	525.54	Joback Method
cpg	280.75	J/molxK	495.65	Joback Method
cpg	268.41	J/molxK	465.76	Joback Method
cpg	325.12	J/molxK	615.20	Joback Method
dvisc	0.0002821	Paxs	435.87	Joback Method
dvisc	0.0003753	Paxs	399.03	Joback Method
dvisc	0.0005291	Paxs	362.20	Joback Method
dvisc	0.0008063	Paxs	325.36	Joback Method
dvisc	0.0013683	Paxs	288.52	Joback Method
dvisc	0.0027108	Paxs	251.69	Joback Method
dvisc	0.0067893	Paxs	214.85	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.56577e+01
Coeff. B	-4.06603e+03
Coeff. C	-6.26780e+01
Temperature range (K), min.	327.22
Temperature range (K), max.	455.68

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2371199&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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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