2-Heptanone, 5-methyl-

Other names: 5-Methyl-2-heptanone
Inchi: InChI=1S/C8H16O/c1-4-7(2)5-6-8(3)9/h7H,4-6H2,1-3H3
InchiKey: WYDAUGNQLUXTFB-UHFFFAOYSA-N
Formula: C8H16O
SMILES: CCC(C)CCC(C)=O
Mol. weight [g/mol]: 128.21
CAS: 18217-12-4

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	971.00		NIST Webbook
rinpol	974.00		NIST Webbook
rinpol	974.00		NIST Webbook
rinpol	971.00		NIST Webbook
ripol	1256.00		NIST Webbook
ripol	1252.00		NIST Webbook
tb	441.00 ± 3.00	K	NIST Webbook
tb	433.00 ± 3.00	K	NIST Webbook
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	1.54335e+01
Coeff. B	-4.00554e+03
Coeff. C	-6.26360e+01
Temperature range (K), min.	327.10
Temperature range (K), max.	458.36

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18217124&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
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
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

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