4-Octanone

Other names:	Butyl propyl ketone
	Propyl n-butyl ketone
	n-C4H9COCH2CH2CH3
	octan-4-one
Inchi:	InChI=1S/C8H16O/c1-3-5-7-8(9)6-4-2/h3-7H2,1-2H3
InchiKey:	YWXLSHOWXZUMSR-UHFFFAOYSA-N
Formula:	C8H16O
SMILES:	CCCCC(=O)CCC
Mol. weight [g/mol]:	128.21
CAS:	589-63-9

Physical Properties

Property code	Value	Unit	Source
chl	-5048.58	kJ/mol	NIST Webbook
gf	-112.44	kJ/mol	Joback Method
hf	-349.30 ± 2.80	kJ/mol	NIST Webbook
hfus	18.07	kJ/mol	Joback Method
hvap	37.10 ± 0.20	kJ/mol	NIST Webbook
ie	9.10 ± 0.05	eV	NIST Webbook
log10ws	-2.45		Crippen Method
logp	2.546		Crippen Method
mcvol	125.150	ml/mol	McGowan Method
pc	2704.22	kPa	Joback Method
rhoc	257.71 ± 2.56	kg/m3	NIST Webbook
rinpol	965.00		NIST Webbook
rinpol	974.00		NIST Webbook
rinpol	975.00		NIST Webbook
rinpol	984.00		NIST Webbook
rinpol	977.00		NIST Webbook
rinpol	953.00		NIST Webbook
rinpol	970.00		NIST Webbook
rinpol	978.00		NIST Webbook
rinpol	959.00		NIST Webbook
rinpol	953.00		NIST Webbook
rinpol	958.00		NIST Webbook
rinpol	958.00		NIST Webbook
ripol	1197.00		NIST Webbook

ripol	1231.00		NIST Webbook
ripol	1236.00		NIST Webbook
ripol	1236.00		NIST Webbook
ripol	1197.00		NIST Webbook
ripol	1224.00		NIST Webbook
ripol	1250.00		NIST Webbook
ripol	1236.00		NIST Webbook
tb	440.00 ± 5.00	K	NIST Webbook
tb	439.00 ± 3.00	K	NIST Webbook
tb	436.00 ± 3.00	K	NIST Webbook
tb	441.00 ± 3.00	K	NIST Webbook
tb	436.00 ± 3.00	K	NIST Webbook
tb	441.00 ± 2.00	K	NIST Webbook
tc	623.80 ± 0.20	K	NIST Webbook
tf	229.85	K	Joback Method
vc	0.489	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.31	J/mol×K	611.72	Joback Method
cpg	255.50	J/mol×K	436.31	Joback Method
cpg	267.99	J/mol×K	465.55	Joback Method
cpg	280.00	J/mol×K	494.78	Joback Method
cpg	291.52	J/mol×K	524.02	Joback Method
cpg	302.57	J/mol×K	553.25	Joback Method
cpg	313.17	J/mol×K	582.49	Joback Method
dvisc	0.0002948	Pa×s	436.31	Joback Method
dvisc	0.0043730	Pa×s	229.85	Joback Method
dvisc	0.0020821	Pa×s	264.26	Joback Method
dvisc	0.0011762	Pa×s	298.67	Joback Method
dvisc	0.0007477	Pa×s	333.08	Joback Method
dvisc	0.0005173	Pa×s	367.49	Joback Method
dvisc	0.0003813	Pa×s	401.90	Joback Method
hvapt	36.40	kJ/mol	360.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47747e+01
Coeff. B	-3.82488e+03
Coeff. C	-6.24000e+01
Temperature range (K), min.	326.42
Temperature range (K), max.	466.58

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=C589639&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

chl:	Standard liquid enthalpy of combustion
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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhoc:	Critical density
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