3-Decanone

Other names:	Decan-3-one
	Ethyl heptyl ketone
	Ethyl n-heptyl ketone
Inchi:	InChI=1S/C10H20O/c1-3-5-6-7-8-9-10(11)4-2/h3-9H2,1-2H3
InchiKey:	XJLDYKIEURAVBW-UHFFFAOYSA-N
Formula:	C10H20O
SMILES:	CCCCCCCC(=O)CC
Mol. weight [g/mol]:	156.27
CAS:	928-80-3

Physical Properties

Property code	Value	Unit	Source
gf	-95.60	kJ/mol	Joback Method
hf	-362.31	kJ/mol	Joback Method
hfus	23.25	kJ/mol	Joback Method
hvap	44.60	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	3.326		Crippen Method
mcvol	153.330	ml/mol	McGowan Method
pc	2235.52	kPa	Joback Method
rhoc	248.46 ± 6.25	kg/m3	NIST Webbook
rinpol	1168.00		NIST Webbook
rinpol	1184.00		NIST Webbook
rinpol	1184.00		NIST Webbook
rinpol	1188.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1184.00		NIST Webbook
rinpol	1176.00		NIST Webbook
rinpol	1187.00		NIST Webbook
rinpol	1177.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1168.00		NIST Webbook
rinpol	1195.00		NIST Webbook
ripol	1455.00		NIST Webbook
ripol	1455.00		NIST Webbook
ripol	1491.00		NIST Webbook

ripol	1455.00		NIST Webbook
tb	484.00 ± 6.00	K	NIST Webbook
tb	477.70	K	NIST Webbook
tb	478.00 ± 3.00	K	NIST Webbook
tc	667.60 ± 0.50	K	NIST Webbook
tf	275.60 ± 4.00	K	NIST Webbook
vc	0.602	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.00	J/mol×K	482.07	Joback Method
cpg	356.42	J/mol×K	510.87	Joback Method
cpg	370.27	J/mol×K	539.66	Joback Method
cpg	383.54	J/mol×K	568.46	Joback Method
cpg	396.27	J/mol×K	597.26	Joback Method
cpg	408.46	J/mol×K	626.06	Joback Method
cpg	420.12	J/mol×K	654.85	Joback Method
dvisc	0.0045381	Pa×s	252.39	Joback Method
dvisc	0.0020766	Pa×s	290.67	Joback Method
dvisc	0.0011399	Pa×s	328.95	Joback Method
dvisc	0.0007090	Pa×s	367.23	Joback Method
dvisc	0.0004824	Pa×s	405.51	Joback Method
dvisc	0.0003508	Pa×s	443.79	Joback Method
dvisc	0.0002683	Pa×s	482.07	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49623e+01
Coeff. B	-4.18082e+03
Coeff. C	-7.35200e+01
Temperature range (K), min.	358.42
Temperature range (K), max.	506.73

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C928803&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
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