6-Undecanone

Other names:	6-Oxoundecane
	Amyl ketone
	Di-N-amyl ketone
	Diamyl ketone
	Dipentyl ketone
	Pentyl ketone
	Undecan-6-one
	Undecanone-(6)
Inchi:	InChI=1S/C11H22O/c1-3-5-7-9-11(12)10-8-6-4-2/h3-10H2,1-2H3
InchiKey:	ZPQAKYPOZRXKFA-UHFFFAOYSA-N
Formula:	C11H22O
SMILES:	CCCCCC(=O)CCCCC
Mol. weight [g/mol]:	170.29
CAS:	927-49-1

Physical Properties

Property code	Value	Unit	Source
chl	-7024.60 ± 1.80	kJ/mol	NIST Webbook
gf	-87.18	kJ/mol	Joback Method
hf	-387.40 ± 2.00	kJ/mol	NIST Webbook
hfl	-448.10 ± 1.90	kJ/mol	NIST Webbook
hfus	25.84	kJ/mol	Joback Method
hvap	63.50 ± 0.50	kJ/mol	NIST Webbook
hvap	60.72 ± 0.50	kJ/mol	NIST Webbook
hvap	59.00	kJ/mol	NIST Webbook
hvap	61.80	kJ/mol	NIST Webbook
log10ws	-3.71		Crippen Method
logp	3.716		Crippen Method
mcvol	167.420	ml/mol	McGowan Method
pc	2045.61	kPa	Joback Method
rhoc	245.22 ± 6.81	kg/m3	NIST Webbook
rinpol	1237.00		NIST Webbook
rinpol	1249.00		NIST Webbook
rinpol	1253.00		NIST Webbook
rinpol	1261.00		NIST Webbook
rinpol	1231.00		NIST Webbook
rinpol	1255.00		NIST Webbook

rinpol	1258.00		NIST Webbook
rinpol	1249.00		NIST Webbook
rinpol	1249.00		NIST Webbook
rinpol	1258.00		NIST Webbook
rinpol	1253.00		NIST Webbook
rinpol	1258.00		NIST Webbook
rinpol	1258.00		NIST Webbook
rinpol	1274.00		NIST Webbook
ripol	1528.00		NIST Webbook
ripol	1528.00		NIST Webbook
ripol	1527.00		NIST Webbook
ripol	1528.00		NIST Webbook
ripol	1528.00		NIST Webbook
tb	501.20	K	NIST Webbook
tb	438.15 ± 15.00	K	NIST Webbook
tb	496.00 ± 4.00	K	NIST Webbook
tb	501.20 ± 0.60	K	NIST Webbook
tb	498.00 ± 5.00	K	NIST Webbook
tb	496.00 ± 5.00	K	NIST Webbook
tc	678.50 ± 1.50	K	NIST Webbook
tf	287.00 ± 3.00	K	NIST Webbook
tf	287.80 ± 4.00	K	NIST Webbook
tf	287.80 ± 2.00	K	NIST Webbook
tf	270.00 ± 10.00	K	NIST Webbook
tf	287.00 ± 4.00	K	NIST Webbook
tf	287.70 ± 1.50	K	NIST Webbook
tf	285.70 ± 3.00	K	NIST Webbook
tf	288.00 ± 3.00	K	NIST Webbook
vc	0.657	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	388.23	J/mol×K	504.95	Joback Method
cpg	403.46	J/mol×K	533.52	Joback Method
cpg	418.07	J/mol×K	562.10	Joback Method
cpg	432.09	J/mol×K	590.67	Joback Method
cpg	445.51	J/mol×K	619.25	Joback Method
cpg	458.36	J/mol×K	647.82	Joback Method
cpg	470.65	J/mol×K	676.40	Joback Method
cpl	362.70	J/mol×K	298.15	NIST Webbook

dvisc	0.0020210	Pa×s	303.88	Joback Method
dvisc	0.0044945	Pa×s	263.66	Joback Method
dvisc	0.0010954	Pa×s	344.09	Joback Method
dvisc	0.0006749	Pa×s	384.30	Joback Method
dvisc	0.0004558	Pa×s	424.52	Joback Method
dvisc	0.0003295	Pa×s	464.74	Joback Method
dvisc	0.0002508	Pa×s	504.95	Joback Method
hvapt	55.30	kJ/mol	465.50	NIST Webbook
hvapt	50.40	kJ/mol	487.00	NIST Webbook
hvapt	45.80	kJ/mol	448.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.61826e+01
Coeff. B	-4.73593e+03
Coeff. C	-8.04700e+01
Temperature range (K), min.	378.42
Temperature range (K), max.	516.11

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C927491&Units=SI

Legend

chl: Standard liquid enthalpy of combustion

cpg: Ideal gas heat capacity

cpl: Liquid phase heat capacity

dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
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