2-Tridecanone

Other names:	2-Tridecankje
	Mathyl undecyl kepoje
	Methyl n-undecyl ketone
	Methyl undecyl ketone
	Tridecan-2-one
	Tridecanone-2
Inchi:	InChI=1S/C13H26O/c1-3-4-5-6-7-8-9-10-11-12-13(2)14/h3-12H2,1-2H3
InchiKey:	CYIFVRUOHKNECG-UHFFFAOYSA-N
Formula:	C13H26O
SMILES:	CCCCCCCCCCCC(C)=O
Mol. weight [g/mol]:	198.34
CAS:	593-08-8

Physical Properties

Property code	Value	Unit	Source
gf	-70.34	kJ/mol	Joback Method
hf	-424.23	kJ/mol	Joback Method
hfus	44.03	kJ/mol	Measurements, Correlations, and Mod. UNIFAC (Do) Prediction of (Solid-Liquid) Phase Equilibria Diagrams in Binary Systems (Aliphatic Ketone + an Alcohol)
hvap	51.28	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	4.496		Crippen Method
mcvol	195.600	ml/mol	McGowan Method
pc	1731.78	kPa	Joback Method
rhoc	241.98 ± 7.93	kg/m3	NIST Webbook
rinpol	1497.30		NIST Webbook
rinpol	1478.00		NIST Webbook
rinpol	1497.00		NIST Webbook
rinpol	1481.00		NIST Webbook
rinpol	1477.00		NIST Webbook
rinpol	1497.00		NIST Webbook
rinpol	1476.00		NIST Webbook
rinpol	1491.00		NIST Webbook
rinpol	1499.00		NIST Webbook

rinpol	1491.00	NIST Webbook
rinpol	1480.00	NIST Webbook
rinpol	1480.00	NIST Webbook
rinpol	1475.00	NIST Webbook
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rinpol	1479.00	NIST Webbook
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rinpol	1500.00	NIST Webbook
rinpol	1489.00	NIST Webbook
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ripol	1816.00	NIST Webbook
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ripol	1814.00	NIST Webbook
ripol	1805.00	NIST Webbook
ripol	1810.00	NIST Webbook
ripol	1806.00	NIST Webbook
ripol	1790.00	NIST Webbook
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ripol	1816.00	NIST Webbook
ripol	1771.00	NIST Webbook
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ripol	1790.00		NIST Webbook
ripol	1791.00		NIST Webbook
ripol	1815.00		NIST Webbook
ripol	1807.00		NIST Webbook
ripol	1801.00		NIST Webbook
ripol	1828.00		NIST Webbook
ripol	1792.00		NIST Webbook
tb	536.15 ± 2.00	K	NIST Webbook
tb	535.90 ± 2.00	K	NIST Webbook
tb	535.65 ± 2.00	K	NIST Webbook
tb	528.15 ± 2.00	K	NIST Webbook
tb	536.20	K	NIST Webbook
tc	717.00 ± 3.00	K	NIST Webbook
tf	286.20	K	Joback Method
vc	0.769	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.60	J/mol×K	607.06	Joback Method
cpg	575.73	J/mol×K	719.75	Joback Method
cpg	562.38	J/mol×K	691.58	Joback Method
cpg	548.43	J/mol×K	663.40	Joback Method
cpg	533.84	J/mol×K	635.23	Joback Method
cpg	486.12	J/mol×K	550.71	Joback Method
cpg	502.70	J/mol×K	578.88	Joback Method

dvisc	0.0018390	Pa×s	330.28	Joback Method
dvisc	0.0009747	Pa×s	374.37	Joback Method
dvisc	0.0005905	Pa×s	418.46	Joback Method
dvisc	0.0003936	Pa×s	462.54	Joback Method
dvisc	0.0002816	Pa×s	506.62	Joback Method
dvisc	0.0042194	Pa×s	286.20	Joback Method
dvisc	0.0002125	Pa×s	550.71	Joback Method
hvapt	62.10	kJ/mol	447.50	NIST Webbook
hvapt	69.80	kJ/mol	383.00	NIST Webbook
hvapt	49.60	kJ/mol	514.00	NIST Webbook
hvapt	61.00	kJ/mol	467.00	NIST Webbook
hvapt	69.60	kJ/mol	434.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	407.20	K	1.30	NIST Webbook
tbrp	433.20	K	2.10	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51705e+01
Coeff. B	-4.70629e+03
Coeff. C	-9.02000e+01
Temperature range (K), min.	406.42
Temperature range (K), max.	567.56

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C593088&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
Solubility of fragrance raw materials in water: Experimental study, correlations, and Mod. UNIFAC (Do) prediction	https://www.doi.org/10.1016/j.jct.2010.07.013
Measurements, Correlations, and Mod. UNIFAC (Do) Prediction of (Solid + Liquid) Phase Equilibria Diagrams in Binary Systems (Aliphatic Ketone + an Alcohol):	https://www.doi.org/10.1021/je100725a
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume