2-Dodecanone

Other names:	Decyl methyl ketone
	Dodecan-2-one
	Dodecanone-(2)
	Methyl decyl ketone
Inchi:	InChI=1S/C12H24O/c1-3-4-5-6-7-8-9-10-11-12(2)13/h3-11H2,1-2H3
InchiKey:	LSKONYYRONEBKA-UHFFFAOYSA-N
Formula:	C12H24O
SMILES:	CCCCCCCCCCC(C)=O
Mol. weight [g/mol]:	184.32
CAS:	6175-49-1

Physical Properties

Property code	Value	Unit	Source
chl	-7676.00 ± 1.70	kJ/mol	NIST Webbook
gf	-78.76	kJ/mol	Joback Method
hf	-404.30 ± 2.50	kJ/mol	NIST Webbook
hfl	-476.10 ± 2.40	kJ/mol	NIST Webbook
hfus	39.48	kJ/mol	Measurements, Correlations, and Mod. UNIFAC (Do) Prediction of (Solid-Liquid) Phase Equilibria Diagrams in Binary Systems (Aliphatic Ketone + an Alcohol)
hvap	71.83	kJ/mol	NIST Webbook
hvap	71.80 ± 0.60	kJ/mol	NIST Webbook
hvap	71.83 ± 0.64	kJ/mol	NIST Webbook
log10ws	-4.13		Crippen Method
logp	4.106		Crippen Method
mcvol	181.510	ml/mol	McGowan Method
pc	1878.90	kPa	Joback Method
rhoc	245.14 ± 7.37	kg/m3	NIST Webbook
rinpol	1373.00		NIST Webbook
rinpol	1356.00		NIST Webbook
rinpol	1361.00		NIST Webbook
rinpol	1384.00		NIST Webbook
rinpol	1377.00		NIST Webbook
rinpol	1370.00		NIST Webbook
rinpol	1379.00		NIST Webbook

rinpol	1378.00	NIST Webbook
rinpol	1380.00	NIST Webbook
rinpol	1401.00	NIST Webbook
rinpol	1345.00	NIST Webbook
rinpol	1388.00	NIST Webbook
rinpol	1389.00	NIST Webbook
rinpol	1375.00	NIST Webbook
rinpol	1402.00	NIST Webbook
rinpol	1396.00	NIST Webbook
rinpol	1373.00	NIST Webbook
rinpol	1389.00	NIST Webbook
rinpol	1375.00	NIST Webbook
rinpol	1367.00	NIST Webbook
rinpol	1395.00	NIST Webbook
rinpol	1404.00	NIST Webbook
rinpol	1397.00	NIST Webbook
rinpol	1404.00	NIST Webbook
rinpol	1410.00	NIST Webbook
rinpol	1410.00	NIST Webbook
rinpol	1377.00	NIST Webbook
rinpol	1370.00	NIST Webbook
rinpol	1377.00	NIST Webbook
rinpol	1377.00	NIST Webbook
rinpol	1379.00	NIST Webbook
rinpol	1388.00	NIST Webbook
rinpol	1373.00	NIST Webbook
rinpol	1371.00	NIST Webbook
rinpol	1395.00	NIST Webbook
rinpol	1410.00	NIST Webbook
rinpol	1348.00	NIST Webbook
rinpol	1375.00	NIST Webbook
rinpol	1375.00	NIST Webbook
rinpol	1371.00	NIST Webbook
rinpol	1366.50	NIST Webbook
rinpol	1382.10	NIST Webbook
rinpol	1383.80	NIST Webbook
rinpol	1394.30	NIST Webbook
rinpol	1392.90	NIST Webbook
rinpol	1391.00	NIST Webbook
ripol	1698.00	NIST Webbook
ripol	1704.00	NIST Webbook
ripol	1692.00	NIST Webbook
ripol	1704.00	NIST Webbook
ripol	1710.00	NIST Webbook

ripol	1711.00		NIST Webbook
ripol	1692.00		NIST Webbook
ripol	1708.00		NIST Webbook
ripol	1709.00		NIST Webbook
ripol	1674.00		NIST Webbook
ripol	1688.00		NIST Webbook
ripol	1698.00		NIST Webbook
ripol	1697.00		NIST Webbook
ripol	1698.00		NIST Webbook
ripol	1692.00		NIST Webbook
ripol	1697.00		NIST Webbook
ripol	1688.00		NIST Webbook
tb	519.65 ± 2.00	K	NIST Webbook
tb	518.15 ± 2.00	K	NIST Webbook
tb	519.65 ± 2.00	K	NIST Webbook
tc	702.10 ± 2.70	K	NIST Webbook
tf	274.93	K	Joback Method
vc	0.714	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.69	J/mol×K	669.65	Joback Method
cpg	482.21	J/mol×K	612.92	Joback Method
cpg	467.55	J/mol×K	584.56	Joback Method
cpg	452.25	J/mol×K	556.19	Joback Method
cpg	436.30	J/mol×K	527.83	Joback Method
cpg	496.25	J/mol×K	641.28	Joback Method
cpg	522.54	J/mol×K	698.01	Joback Method
dvisc	0.0043838	Pa×s	274.93	Joback Method
dvisc	0.0002319	Pa×s	527.83	Joback Method
dvisc	0.0003061	Pa×s	485.68	Joback Method
dvisc	0.0004257	Pa×s	443.53	Joback Method
dvisc	0.0006347	Pa×s	401.38	Joback Method
dvisc	0.0010391	Pa×s	359.23	Joback Method
dvisc	0.0019395	Pa×s	317.08	Joback Method
hvapt	48.10	kJ/mol	497.50	NIST Webbook
hvapt	61.10	kJ/mol	435.00	NIST Webbook
hvapt	60.80	kJ/mol	497.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51720e+01
Coeff. B	-4.58012e+03
Coeff. C	-8.56680e+01
Temperature range (K), min.	393.38
Temperature range (K), max.	550.16

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6175491&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
Measurements, Correlations, and Mod.	https://www.doi.org/10.1021/je100725a
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
UNIFAC (Do) Prediction of (Solid-Liquid) Phase Equilibria Diagrams in Binary Systems (Aliphatic Ketone + an Alcohol):	http://link.springer.com/article/10.1007/BF02311772
McGowan Method:	

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
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

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