

2-Adamantanone

Other names:	2-Adamantone 2-Oxoadamantane Adamantan-2-one Tricyclo[3.3.1.1(3,7)]decanone adamantanone tricyclo[3.3.1.13,7]decan-2-one
Inchi:	InChI=1S/C10H14O/c11-10-8-2-6-1-7(4-8)5-9(10)3-6/h6-9H,1-5H2
InchiKey:	IYKFYARMMIESOX-UHFFFAOYSA-N
Formula:	C10H14O
SMILES:	O=C1C2CC3CC(C2)CC1C3
Mol. weight [g/mol]:	150.22
CAS:	700-58-3

Physical Properties

Property code	Value	Unit	Source
chs	-5625.00 ± 4.00	kJ/mol	NIST Webbook
gf	73.17	kJ/mol	Joback Method
hf	-231.00 ± 4.60	kJ/mol	NIST Webbook
hfs	-311.00 ± 4.00	kJ/mol	NIST Webbook
hfus	7.63	kJ/mol	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
hfus	11.77	kJ/mol	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
hsub	76.10 ± 1.50	kJ/mol	NIST Webbook
hsub	66.40 ± 0.30	kJ/mol	NIST Webbook
hsub	80.30 ± 2.50	kJ/mol	NIST Webbook
hsub	80.00 ± 3.00	kJ/mol	NIST Webbook
hsub	66.30 ± 0.80	kJ/mol	NIST Webbook
hvap	60.70 ± 0.20	kJ/mol	NIST Webbook
ie	8.67	eV	NIST Webbook
ie	8.59	eV	NIST Webbook
ie	8.76	eV	NIST Webbook
ie	8.62	eV	NIST Webbook
ie	8.80 ± 0.02	eV	NIST Webbook
log10ws	-2.01		Crippen Method

logp	2.012		Crippen Method
mcvol	120.750	ml/mol	McGowan Method
pc	3224.64	kPa	Joback Method
rinpol	1379.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1320.00		NIST Webbook
rinpol	1391.00		NIST Webbook
rinpol	1360.00		NIST Webbook
rinpol	1320.00		NIST Webbook
rinpol	1344.00		NIST Webbook
rinpol	1357.00		NIST Webbook
rinpol	1320.00		NIST Webbook
rinpol	1332.00		NIST Webbook
rinpol	1370.00		NIST Webbook
rinpol	1332.00		NIST Webbook
ripol	1895.00		NIST Webbook
ripol	1918.00		NIST Webbook
ripol	1867.00		NIST Webbook
tb	515.84	K	Joback Method
tc	746.98	K	Joback Method
tf	316.74	K	Joback Method
tt	557.50	K	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
tt	216.40	K	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
vc	0.465	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.43	J/mol×K	515.84	Joback Method
cpg	396.28	J/mol×K	708.46	Joback Method
cpg	381.43	J/mol×K	669.93	Joback Method
cpg	365.50	J/mol×K	631.41	Joback Method
cpg	410.13	J/mol×K	746.98	Joback Method
cpg	330.08	J/mol×K	554.36	Joback Method
cpg	348.41	J/mol×K	592.89	Joback Method

cpl	359.00	J/mol×K	557.50	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cpl	394.00	J/mol×K	610.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cpl	381.00	J/mol×K	590.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cpl	367.00	J/mol×K	570.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	101.90	J/mol×K	170.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	11.78	J/mol×K	20.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	5.82	J/mol×K	15.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	24.08	J/mol×K	30.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	29.25	J/mol×K	35.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	33.72	J/mol×K	40.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states

cps	37.58	J/mol×K	45.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	40.93	J/mol×K	50.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	46.54	J/mol×K	60.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	51.40	J/mol×K	70.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	56.13	J/mol×K	80.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	65.70	J/mol×K	100.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	60.88	J/mol×K	90.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	70.62	J/mol×K	110.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	75.56	J/mol×K	120.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	80.56	J/mol×K	130.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states

cps	85.65	J/mol×K	140.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	90.88	J/mol×K	150.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	96.28	J/mol×K	160.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	1.66	J/mol×K	10.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	107.70	J/mol×K	180.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	113.90	J/mol×K	190.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	120.50	J/mol×K	200.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	127.70	J/mol×K	210.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	132.60	J/mol×K	216.40	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	144.00	J/mol×K	216.40	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states

cps	146.20	J/mol×K	220.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	152.30	J/mol×K	230.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	248.00	J/mol×K	380.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	164.80	J/mol×K	250.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	171.20	J/mol×K	260.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	359.00	J/mol×K	557.50	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	347.00	J/mol×K	540.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	334.00	J/mol×K	520.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	322.00	J/mol×K	500.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	309.00	J/mol×K	480.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states

cps	297.00	J/mol×K	460.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	285.00	J/mol×K	440.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	272.00	J/mol×K	420.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	260.00	J/mol×K	400.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	158.50	J/mol×K	240.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	236.00	J/mol×K	360.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	224.00	J/mol×K	340.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	211.00	J/mol×K	320.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	197.80	J/mol×K	300.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	196.60	J/mol×K	298.15	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states

cps	191.00	J/mol×K	290.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	184.30	J/mol×K	280.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	177.70	J/mol×K	270.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
cps	18.17	J/mol×K	25.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
hfust	11.77	kJ/mol	557.50	NIST Webbook
hvapt	65.80	kJ/mol	313.70	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
psub	0.03	kPa	332.90	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
psub	8.98e-03	kPa	318.18	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
psub	7.40e-03	kPa	315.72	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
psub	7.67e-03	kPa	315.71	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
psub	6.09e-03	kPa	313.26	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states

psub	6.07e-03	kPa	313.24	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
psub	4.99e-03	kPa	310.80	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
psub	5.22e-03	kPa	310.80	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
psub	4.11e-03	kPa	308.33	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
psub	2.65e-03	kPa	303.32	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
psub	1.75e-03	kPa	298.39	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
psub	1.43e-03	kPa	295.94	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
psub	1.39e-03	kPa	295.90	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
psub	1.11e-03	kPa	293.48	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
psub	1.10e-03	kPa	293.34	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states

psub	6.86e-04	kPa	288.42	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
psub	4.18e-04	kPa	283.47	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
psub	2.92e-04	kPa	280.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
psub	0.01	kPa	323.06	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
psub	0.31	kPa	373.40	Adamantanes: Benchmarking of thermochemical properties
psub	0.25	kPa	368.40	Adamantanes: Benchmarking of thermochemical properties
psub	0.02	kPa	327.99	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
psub	0.13	kPa	358.30	Adamantanes: Benchmarking of thermochemical properties
psub	0.10	kPa	353.30	Adamantanes: Benchmarking of thermochemical properties
psub	0.08	kPa	348.40	Adamantanes: Benchmarking of thermochemical properties
psub	0.05	kPa	343.30	Adamantanes: Benchmarking of thermochemical properties
psub	0.04	kPa	338.50	Adamantanes: Benchmarking of thermochemical properties

psub	0.03	kPa	333.40	Adamantanes: Benchmarking of thermochemical properties
psub	0.01	kPa	323.40	Adamantanes: Benchmarking of thermochemical properties
psub	9.03e-03	kPa	318.40	Adamantanes: Benchmarking of thermochemical properties
psub	6.08e-03	kPa	313.40	Adamantanes: Benchmarking of thermochemical properties
psub	4.17e-03	kPa	308.40	Adamantanes: Benchmarking of thermochemical properties
psub	3.41e-03	kPa	306.40	Adamantanes: Benchmarking of thermochemical properties
psub	2.58e-03	kPa	303.40	Adamantanes: Benchmarking of thermochemical properties
psub	1.99e-03	kPa	300.40	Adamantanes: Benchmarking of thermochemical properties
psub	1.72e-03	kPa	298.50	Adamantanes: Benchmarking of thermochemical properties
psub	1.56e-03	kPa	297.40	Adamantanes: Benchmarking of thermochemical properties
psub	1.42e-03	kPa	296.40	Adamantanes: Benchmarking of thermochemical properties
psub	1.09e-03	kPa	293.50	Adamantanes: Benchmarking of thermochemical properties
psub	0.02	kPa	328.40	Adamantanes: Benchmarking of thermochemical properties
psub	0.18	kPa	363.40	Adamantanes: Benchmarking of thermochemical properties

sml	448.00	J/mol×K	610.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sml	414.00	J/mol×K	557.50	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sml	423.00	J/mol×K	570.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sml	435.00	J/mol×K	590.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	213.00	J/mol×K	280.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	344.00	J/mol×K	480.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	331.00	J/mol×K	460.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	318.00	J/mol×K	440.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	305.00	J/mol×K	420.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	291.80	J/mol×K	400.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states

sms	278.70	J/mol×K	380.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	265.60	J/mol×K	360.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	252.50	J/mol×K	340.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	239.30	J/mol×K	320.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	226.10	J/mol×K	300.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	224.90	J/mol×K	298.15	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	219.50	J/mol×K	290.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	206.40	J/mol×K	270.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	199.80	J/mol×K	260.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	193.20	J/mol×K	250.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states

sms	186.60	J/mol×K	240.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	180.00	J/mol×K	230.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	173.40	J/mol×K	220.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	171.00	J/mol×K	216.40	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	135.70	J/mol×K	216.40	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	131.80	J/mol×K	210.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	125.80	J/mol×K	200.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	119.80	J/mol×K	190.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	113.80	J/mol×K	180.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	107.80	J/mol×K	170.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states

sms	101.80	J/mol×K	160.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	95.74	J/mol×K	150.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	89.65	J/mol×K	140.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	83.50	J/mol×K	130.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	77.25	J/mol×K	120.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	64.40	J/mol×K	100.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	57.74	J/mol×K	90.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	50.86	J/mol×K	80.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	43.68	J/mol×K	70.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	36.14	J/mol×K	60.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states

sms	28.16	J/molxK	50.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	24.03	J/molxK	45.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	19.83	J/molxK	40.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	15.62	J/molxK	35.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	11.51	J/molxK	30.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	7.67	J/molxK	25.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	4.35	J/molxK	20.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	1.89	J/molxK	15.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	0.51	J/molxK	10.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	356.00	J/molxK	500.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states

sms	369.00	J/mol×K	520.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	382.00	J/mol×K	540.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	393.00	J/mol×K	557.50	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states
sms	70.90	J/mol×K	110.00	Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Adamantanes: Benchmarking of thermochemical properties:	https://www.doi.org/10.1016/j.jct.2016.05.017
Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states:	https://www.doi.org/10.1016/j.tca.2006.08.018
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=C700583&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions

hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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
psub:	Sublimation pressure
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
sml:	Liquid phase molar entropy
sms:	Solid phase molar entropy
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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