Adamantane

Other names:	4,7-methano-1H-indene, octahydro-, (3a.alpha.,4.beta.,7.beta.,7a.alpha.)- 4,7-methanoindan, hexahydro-, exo- JP-10 Tricyclo(3,3,1,1, exo-3,4,8,9-tetrahydrodicyclopentadiene exo-5,6-trimethylenenorbornane exo-octahydro-4,7-methano-1H-indene exo-tetrahydrobicyclopentadiene exo-tetrahydrodicyclopentadiene exo-tricyclo[5.2.1.02,6]decane exo-trimethylenenorbornane jp10 tricyclo[3.3.1.1(3,7)]decane
Inchi:	InChI=1S/C10H16/c1-7-2-9-4-8(1)5-10(3-7)6-9/h7-10H,1-6H2
InchiKey:	ORILYTVJVMAKLC-UHFFFAOYSA-N
Formula:	C10H16
SMILES:	C1C2CC3CC1CC(C2)C3
Mol. weight [g/mol]:	136.23
CAS:	281-23-2

Physical Properties

Property code	Value	Unit	Source
chs	-6033.10 ± 2.80	kJ/mol	NIST Webbook
chs	-6033.40 ± 3.30	kJ/mol	NIST Webbook
chs	-6024.50 ± 0.71	kJ/mol	NIST Webbook
chs	-6029.00 ± 4.00	kJ/mol	NIST Webbook
gf	195.76	kJ/mol	Joback Method
hf	-137.90 ± 0.79	kJ/mol	NIST Webbook
hf	-129.00 ± 4.00	kJ/mol	NIST Webbook
hf	-133.60 ± 2.50	kJ/mol	NIST Webbook
hf	-138.70	kJ/mol	NIST Webbook
hf	-134.40 ± 2.30	kJ/mol	NIST Webbook
hfs	-192.50 ± 0.40	kJ/mol	NIST Webbook
hfs	-188.40 ± 3.30	kJ/mol	NIST Webbook
hfs	-193.80	kJ/mol	NIST Webbook
hfs	-188.70 ± 2.80	kJ/mol	NIST Webbook
hfs	-197.20 ± 0.79	kJ/mol	NIST Webbook

hfus	3.09	kJ/mol	Redetermination of the thermodynamic properties of the solid solid transition of adamantane by adiabatic calorimetry to investigate the suitability as a reference material for low-temperature DSC-calibration
hvap	51.70	kJ/mol	NIST Webbook
hvap	48.20	kJ/mol	NIST Webbook
ie	9.75 ± 0.02	eV	NIST Webbook
ie	9.25	eV	NIST Webbook
ie	9.23	eV	NIST Webbook
ie	9.10 ± 0.05	eV	NIST Webbook
ie	9.30 ± 0.10	eV	NIST Webbook
ie	9.31 ± 0.01	eV	NIST Webbook
ie	9.30 ± 0.01	eV	NIST Webbook
ie	9.22	eV	NIST Webbook
ie	9.55	eV	NIST Webbook
ie	9.25	eV	NIST Webbook
ie	9.75	eV	NIST Webbook
ie	9.75	eV	NIST Webbook
ie	9.28	eV	NIST Webbook
ie	9.25 ± 0.04	eV	NIST Webbook
ie	9.20	eV	NIST Webbook
log10ws	-2.73		Crippen Method
logp	2.833		Crippen Method
mcvol	119.180	ml/mol	McGowan Method
pc	3100.18	kPa	Joback Method
rinpol	1120.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1153.00		NIST Webbook
rinpol	1123.00		NIST Webbook
rinpol	1123.00		NIST Webbook
rinpol	1076.00		NIST Webbook
rinpol	1118.00		NIST Webbook
rinpol	1118.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1076.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1114.00		NIST Webbook
rinpol	1104.00		NIST Webbook
rinpol	1095.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1131.00		NIST Webbook
rinpol	1128.00		NIST Webbook

rinpol	1125.00		NIST Webbook
rinpol	1120.00		NIST Webbook
rinpol	1117.00		NIST Webbook
rinpol	1116.00		NIST Webbook
rinpol	1114.00		NIST Webbook
rinpol	1104.00		NIST Webbook
rinpol	1095.00		NIST Webbook
rinpol	1116.00		NIST Webbook
rinpol	1118.00		NIST Webbook
rinpol	1120.00		NIST Webbook
rinpol	1117.00		NIST Webbook
rinpol	1113.00		NIST Webbook
rinpol	1095.20		NIST Webbook
rinpol	1135.30		NIST Webbook
rinpol	1149.00		NIST Webbook
rinpol	1116.00		NIST Webbook
rinpol	1116.00		NIST Webbook
rinpol	1149.00		NIST Webbook
rinpol	1120.00		NIST Webbook
rinpol	1120.00		NIST Webbook
rinpol	1117.00		NIST Webbook
rinpol	1121.00		NIST Webbook
rinpol	1136.90		NIST Webbook
rinpol	1118.00		NIST Webbook
rinpol	1116.00		NIST Webbook
ripol	1400.00		NIST Webbook
ripol	1363.00		NIST Webbook
ripol	1400.00		NIST Webbook
ripol	1363.00		NIST Webbook
ripol	1339.00		NIST Webbook
ripol	1320.00		NIST Webbook
ripol	1363.00		NIST Webbook
ripol	1325.00		NIST Webbook
ripol	1325.00		NIST Webbook
ripol	1400.00		NIST Webbook
ss	195.83	J/mol×K	NIST Webbook
ss	195.83	J/mol×K	NIST Webbook
tb	448.02	K	Joback Method
tc	661.62	K	Joback Method
tf	542.15 ± 1.00	K	NIST Webbook
tf	552.00 ± 3.00	K	NIST Webbook
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.54	J/mol×K	448.02	Joback Method
cpg	293.60	J/mol×K	483.62	Joback Method
cpg	313.20	J/mol×K	519.22	Joback Method
cpg	331.44	J/mol×K	554.82	Joback Method
cpg	348.41	J/mol×K	590.42	Joback Method
cpg	364.21	J/mol×K	626.02	Joback Method
cpg	378.92	J/mol×K	661.62	Joback Method
cps	189.74	J/mol×K	298.15	NIST Webbook
cps	189.74	J/mol×K	298.15	NIST Webbook
dvisc	0.0006121	Pa×s	248.52	Joback Method
dvisc	0.0007158	Pa×s	281.77	Joback Method
dvisc	0.0008100	Pa×s	315.02	Joback Method
dvisc	0.0008951	Pa×s	348.27	Joback Method
dvisc	0.0009721	Pa×s	381.52	Joback Method
dvisc	0.0010419	Pa×s	414.77	Joback Method
dvisc	0.0011052	Pa×s	448.02	Joback Method
hfust	10.90	kJ/mol	541.20	NIST Webbook
hfust	10.90	kJ/mol	541.00	NIST Webbook
hfust	13.80	kJ/mol	543.20	NIST Webbook
hsubt	53.60	kJ/mol	339.00	NIST Webbook
hsubt	58.30	kJ/mol	308.00	NIST Webbook
hsubt	59.70	kJ/mol	323.00	NIST Webbook
hsubt	55.30	kJ/mol	350.50	NIST Webbook
hsubt	54.30	kJ/mol	413.00	NIST Webbook
hsubt	59.70 ± 0.80	kJ/mol	323.00	NIST Webbook
hsubt	59.50	kJ/mol	360.50	NIST Webbook
hsubt	59.30 ± 0.20	kJ/mol	323.00	NIST Webbook
hsubt	58.60 ± 0.60	kJ/mol	333.00	NIST Webbook
rhol	888.34	kg/m3	353.15	Density, Viscosity, Surface Tension, and Refractive Index for Binary Mixtures of 1,3-Dimethyladamantane with Four C10 Alkanes

rhol	935.74	kg/m3	293.15	Density, Viscosity, Surface Tension, and Refractive Index for Binary Mixtures of 1,3-Dimethyladamantane with Four C10 Alkanes
rhol	931.86	kg/m3	298.15	Density, Viscosity, Surface Tension, and Refractive Index for Binary Mixtures of 1,3-Dimethyladamantane with Four C10 Alkanes
rhol	927.95	kg/m3	303.15	Density, Viscosity, Surface Tension, and Refractive Index for Binary Mixtures of 1,3-Dimethyladamantane with Four C10 Alkanes
rhol	920.13	kg/m3	313.15	Density, Viscosity, Surface Tension, and Refractive Index for Binary Mixtures of 1,3-Dimethyladamantane with Four C10 Alkanes
rhol	912.14	kg/m3	323.15	Density, Viscosity, Surface Tension, and Refractive Index for Binary Mixtures of 1,3-Dimethyladamantane with Four C10 Alkanes
rhol	904.25	kg/m3	333.15	Density, Viscosity, Surface Tension, and Refractive Index for Binary Mixtures of 1,3-Dimethyladamantane with Four C10 Alkanes
rhol	880.32	kg/m3	363.15	Density, Viscosity, Surface Tension, and Refractive Index for Binary Mixtures of 1,3-Dimethyladamantane with Four C10 Alkanes

rhol	896.32	kg/m3	343.15	Density, Viscosity, Surface Tension, and Refractive Index for Binary Mixtures of 1,3-Dimethyladamantane with Four C10 Alkanes

Sources

Redetermination of the thermodynamic properties of the solid solid transition of adamantane by adiabatic calorimetry to investigate the suitability as a reference material for low-temperature DSC calibration:	https://www.doi.org/10.1016/j.tca.2006.02.036
Infinite dilution activity coefficients, specific retention volumes and solvation thermodynamics of organic solutes in C78H158 branched alkane solvent:	https://www.doi.org/10.1016/j.fluid.2006.07.015
Density, Viscosity, Surface Tension, and Refractive Index for Binary Mixtures of 1,3-Dimethyladamantane with Four C10 Alkanes:	https://www.doi.org/10.1021/je4008926
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C281232&Units=SI
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubilities of Adamantane and Diamantane in Pressurized Hot Water:	https://www.doi.org/10.1021/je700709m
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Solubility of Adamantane in Phosphonium-Based Ionic Liquids:	https://www.doi.org/10.1021/je9006772
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
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
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure

rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume