Adamantane, 1,3-dimethyl-

Other names:	1,3-dimethyladamantane
	1,3-dimethyltricyclo[3.3.1.1(3,7)]decane
	1,3-dimethyltricyclo[3.3.1.13,7]decane
	tricyclo[3.3.1.1(3,7)]decane, 1,3-dimethyl-
Inchi:	InChI=1S/C12H20/c1-11-4-9-3-10(5-11)7-12(2,6-9)8-11/h9-10H,3-8H2,1-2H3
InchiKey:	CWNOIUTVJRWADX-UHFFFAOYSA-N
Formula:	C12H20
SMILES:	CC12CC3CC(C1)CC(C)(C3)C2
Mol. weight [g/mol]:	164.29
CAS:	702-79-4

Physical Properties

Property code	Value	Unit	Source
chs	-7294.00 ± 3.00	kJ/mol	NIST Webbook
gf	201.62	kJ/mol	Joback Method
hf	-219.00 ± 3.00	kJ/mol	NIST Webbook
hfs	-287.00 ± 3.00	kJ/mol	NIST Webbook
hfus	7.62	kJ/mol	Joback Method
hsub	68.00 ± 1.00	kJ/mol	NIST Webbook
hsub	68.00	kJ/mol	NIST Webbook
hsub	67.80 ± 1.30	kJ/mol	NIST Webbook
hvap	49.70 ± 0.20	kJ/mol	NIST Webbook
hvap	49.40 ± 0.30	kJ/mol	NIST Webbook
ie	9.15	eV	NIST Webbook
log10ws	-3.56		Crippen Method
logp	3.613		Crippen Method
mcvol	147.360	ml/mol	McGowan Method
pc	3000.00 ± 250.00	kPa	NIST Webbook
rhoc	287.50 ± 11.99	kg/m3	NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1184.00		NIST Webbook
rinpol	1184.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1174.00		NIST Webbook
rinpol	1130.00		NIST Webbook

rinpol	1136.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1163.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1154.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1136.00		NIST Webbook
rinpol	1154.00		NIST Webbook
rinpol	1194.00		NIST Webbook
rinpol	1184.00		NIST Webbook
ripol	1296.00		NIST Webbook
ripol	1296.00		NIST Webbook
ripol	1331.00		NIST Webbook
ripol	1310.00		NIST Webbook
tb	471.00 ± 4.00	K	NIST Webbook
tc	708.00 ± 2.00	K	NIST Webbook
tf	245.00 ± 0.50	K	NIST Webbook
vc	0.566	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	479.22	J/mol×K	720.37	Joback Method
cpg	390.80	J/mol×K	531.94	Joback Method
cpg	411.27	J/mol×K	569.63	Joback Method
cpg	430.04	J/mol×K	607.31	Joback Method
cpg	447.41	J/mol×K	645.00	Joback Method
cpg	463.70	J/mol×K	682.68	Joback Method
cpg	368.32	J/mol×K	494.26	Joback Method
hfust	7.36	kJ/mol	221.00	NIST Webbook
hfust	0.92	kJ/mol	245.00	NIST Webbook
hfust	0.94	kJ/mol	244.00	NIST Webbook
hfust	1.54	kJ/mol	190.50	NIST Webbook
hfust	0.92	kJ/mol	245.00	NIST Webbook
hvapt	36.40 ± 0.30	kJ/mol	439.00	NIST Webbook
hvapt	43.70 ± 0.30	kJ/mol	439.00	NIST Webbook
hvapt	45.90 ± 0.30	kJ/mol	439.00	NIST Webbook
hvapt	39.10 ± 0.30	kJ/mol	439.00	NIST Webbook

hvapt	41.50 ± 0.30	kJ/mol	439.00	NIST Webbook
hvapt	49.20 ± 0.20	kJ/mol	308.00	NIST Webbook
rhol	876.55	kg/m3	328.15	Density and Viscosity of Ternary Mixture of Cyclopentanol + exo-Tetrahydrodicyclopentadiene + 1,3-Dimethyladamantane
rhol	872.96	kg/m3	333.15	Density and Viscosity of Ternary Mixture of Cyclopentanol + exo-Tetrahydrodicyclopentadiene + 1,3-Dimethyladamantane
rhol	901.65	kg/m3	293.15	Density, Viscosity, Surface Tension, and Refractive Index for Binary Mixtures of 1,3-Dimethyladamantane with Four C10 Alkanes
rhol	898.09	kg/m3	298.15	Density, Viscosity, Surface Tension, and Refractive Index for Binary Mixtures of 1,3-Dimethyladamantane with Four C10 Alkanes
rhol	894.53	kg/m3	303.15	Density, Viscosity, Surface Tension, and Refractive Index for Binary Mixtures of 1,3-Dimethyladamantane with Four C10 Alkanes
rhol	880.13	kg/m3	323.15	Density and Viscosity of Ternary Mixture of Cyclopentanol + exo-Tetrahydrodicyclopentadiene + 1,3-Dimethyladamantane
rhol	880.17	kg/m3	323.15	Density, Viscosity, Surface Tension, and Refractive Index for Binary Mixtures of 1,3-Dimethyladamantane with Four C10 Alkanes

rhol	872.99	kg/m3	333.15	Density, Viscosity, Surface Tension, and Refractive Index for Binary Mixtures of 1,3-Dimethyladamantane with Four C10 Alkanes
rhol	865.77	kg/m3	343.15	Density, Viscosity, Surface Tension, and Refractive Index for Binary Mixtures of 1,3-Dimethyladamantane with Four C10 Alkanes
rhol	858.52	kg/m3	353.15	Density, Viscosity, Surface Tension, and Refractive Index for Binary Mixtures of 1,3-Dimethyladamantane with Four C10 Alkanes
rhol	851.23	kg/m3	363.15	Density, Viscosity, Surface Tension, and Refractive Index for Binary Mixtures of 1,3-Dimethyladamantane with Four C10 Alkanes
rhol	901.58	kg/m3	293.15	Density, Viscosity, Refractive Index, and Surface Tension for Six Binary Systems of Adamantane Derivatives with 1-Heptanol and Cyclohexylmethanol
rhol	898.04	kg/m3	298.15	Density, Viscosity, Refractive Index, and Surface Tension for Six Binary Systems of Adamantane Derivatives with 1-Heptanol and Cyclohexylmethanol

rhol	894.48	kg/m3	303.15	Density, Viscosity, Refractive Index, and Surface Tension for Six Binary Systems of Adamantane Derivatives with 1-Heptanol and Cyclohexylmethanol
rhol	890.92	kg/m3	308.15	Density, Viscosity, Refractive Index, and Surface Tension for Six Binary Systems of Adamantane Derivatives with 1-Heptanol and Cyclohexylmethanol
rhol	887.35	kg/m3	313.15	Density, Viscosity, Refractive Index, and Surface Tension for Six Binary Systems of Adamantane Derivatives with 1-Heptanol and Cyclohexylmethanol
rhol	883.77	kg/m3	318.15	Density, Viscosity, Refractive Index, and Surface Tension for Six Binary Systems of Adamantane Derivatives with 1-Heptanol and Cyclohexylmethanol
rhol	880.19	kg/m3	323.15	Density, Viscosity, Refractive Index, and Surface Tension for Six Binary Systems of Adamantane Derivatives with 1-Heptanol and Cyclohexylmethanol
rhol	876.60	kg/m3	328.15	Density, Viscosity, Refractive Index, and Surface Tension for Six Binary Systems of Adamantane Derivatives with 1-Heptanol and Cyclohexylmethanol

rhol	873.01	kg/m3	333.15	Density, Viscosity, Refractive Index, and Surface Tension for Six Binary Systems of Adamantane Derivatives with 1-Heptanol and Cyclohexylmethanol
rhol	901.57	kg/m3	293.15	Density and Viscosity of Ternary Mixture of Cyclopentanol + exo-Tetrahydrodicyclopentadiene + 1,3-Dimethyladamantane
rhol	898.00	kg/m3	298.15	Density and Viscosity of Ternary Mixture of Cyclopentanol + exo-Tetrahydrodicyclopentadiene + 1,3-Dimethyladamantane
rhol	883.71	kg/m3	318.15	Density and Viscosity of Ternary Mixture of Cyclopentanol + exo-Tetrahydrodicyclopentadiene + 1,3-Dimethyladamantane
rhol	887.29	kg/m3	313.15	Density and Viscosity of Ternary Mixture of Cyclopentanol + exo-Tetrahydrodicyclopentadiene + 1,3-Dimethyladamantane
rhol	890.86	kg/m3	308.15	Density and Viscosity of Ternary Mixture of Cyclopentanol + exo-Tetrahydrodicyclopentadiene + 1,3-Dimethyladamantane
rhol	894.43	kg/m3	303.15	Density and Viscosity of Ternary Mixture of Cyclopentanol + exo-Tetrahydrodicyclopentadiene + 1,3-Dimethyladamantane

rhol	887.41	kg/m3	313.15	Density, Viscosity, Surface Tension, and Refractive Index for Binary Mixtures of 1,3-Dimethyladamantane with Four C10 Alkanes
sfust	3.76	J/mol×K	245.00	NIST Webbook
sfust	33.30	J/mol×K	221.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C702794&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Density and Viscosity of Ternary Mixture of Cyclopentanol + exo-Tetrahydrodicyclopentadiene + 1,3-Dimethyladamantane:	https://www.doi.org/10.1021/acs.jced.9b00074
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
Density, Viscosity, Refractive Index, and Surface Tension for Six Binary Systems of Adamantane Derivatives with 1-Heptanol and Cyclohexylmethanol:	https://www.doi.org/10.1021/je500381c
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas 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
rhoc:	Critical density

rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume