1,3,5-Trimethyladamantane

Other names:	1,3,5-trimethyl-tricyclo[3.3.1.1(3,7)]decane 1,3,5-trimethyltricyclo[3.3.1.1(3,7)]decane adamantane, 1,3,5-trimethyl- tricyclo[3.3.1.1(3,7)]decane, 1,3,5-trimethyl-
Inchi:	InChI=1S/C13H22/c1-11-4-10-5-12(2,7-11)9-13(3,6-10)8-11/h10H,4-9H2,1-3H3
InchiKey:	WCACLGXPFTYVEL-UHFFFAOYSA-N
Formula:	C13H22
SMILES:	CC12CC3CC(C)(C1)CC(C)(C3)C2
Mol. weight [g/mol]:	178.31
CAS:	707-35-7

Physical Properties

Property code	Value	Unit	Source
chs	-7927.40 ± 4.20	kJ/mol	NIST Webbook
gf	204.55	kJ/mol	Joback Method
hf	-255.00 ± 4.20	kJ/mol	NIST Webbook
hfs	-333.00 ± 4.20	kJ/mol	NIST Webbook
hfus	3.91	kJ/mol	Joback Method
hsub	77.80 ± 1.30	kJ/mol	NIST Webbook
hsub	78.00 ± 1.00	kJ/mol	NIST Webbook
hsub	78.00	kJ/mol	NIST Webbook
hvap	51.70 ± 0.20	kJ/mol	NIST Webbook
log10ws	-3.98		Crippen Method
logp	4.003		Crippen Method
mcvol	161.450	ml/mol	McGowan Method
pc	2632.55	kPa	Joback Method
rinpol	1157.00		NIST Webbook
rinpol	1185.00		NIST Webbook
rinpol	1194.00		NIST Webbook
rinpol	1163.00		NIST Webbook
rinpol	1163.00		NIST Webbook
rinpol	1194.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1148.00		NIST Webbook
rinpol	1152.00		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1163.00		NIST Webbook

rinpol	1153.00		NIST Webbook
rinpol	1161.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1148.00		NIST Webbook
rinpol	1152.00		NIST Webbook
rinpol	1157.00		NIST Webbook
rinpol	1147.00		NIST Webbook
rinpol	1204.00		NIST Webbook
rinpol	1153.00		NIST Webbook
rinpol	1161.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1163.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1128.00		NIST Webbook
ripol	1274.00		NIST Webbook
ripol	1310.00		NIST Webbook
ripol	1292.00		NIST Webbook
tb	517.38	K	Joback Method
tc	749.29	K	Joback Method
tf	253.60 ± 0.20	K	NIST Webbook
vc	0.620	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.44	J/mol×K	517.38	Joback Method
cpg	440.13	J/mol×K	556.03	Joback Method
cpg	460.69	J/mol×K	594.68	Joback Method
cpg	479.58	J/mol×K	633.33	Joback Method
cpg	497.24	J/mol×K	671.98	Joback Method
cpg	514.10	J/mol×K	710.64	Joback Method
cpg	530.62	J/mol×K	749.29	Joback Method
hfust	1.73	kJ/mol	253.60	NIST Webbook
hfust	6.30	kJ/mol	228.20	NIST Webbook
hfust	1.73	kJ/mol	253.60	NIST Webbook

rhol	887.48	kg/m3	293.15	Density, Viscosity, Refractive Index, and Surface Tension for Six Binary Systems of Adamantane Derivatives with 1-Heptanol and Cyclohexylmethanol
rhol	883.99	kg/m3	298.15	Density, Viscosity, Refractive Index, and Surface Tension for Six Binary Systems of Adamantane Derivatives with 1-Heptanol and Cyclohexylmethanol
rhol	880.47	kg/m3	303.15	Density, Viscosity, Refractive Index, and Surface Tension for Six Binary Systems of Adamantane Derivatives with 1-Heptanol and Cyclohexylmethanol
rhol	876.94	kg/m3	308.15	Density, Viscosity, Refractive Index, and Surface Tension for Six Binary Systems of Adamantane Derivatives with 1-Heptanol and Cyclohexylmethanol
rhol	873.40	kg/m3	313.15	Density, Viscosity, Refractive Index, and Surface Tension for Six Binary Systems of Adamantane Derivatives with 1-Heptanol and Cyclohexylmethanol
rhol	869.86	kg/m3	318.15	Density, Viscosity, Refractive Index, and Surface Tension for Six Binary Systems of Adamantane Derivatives with 1-Heptanol and Cyclohexylmethanol

rhol	866.31	kg/m3	323.15	Density, Viscosity, Refractive Index, and Surface Tension for Six Binary Systems of Adamantane Derivatives with 1-Heptanol and Cyclohexylmethanol
rhol	862.76	kg/m3	328.15	Density, Viscosity, Refractive Index, and Surface Tension for Six Binary Systems of Adamantane Derivatives with 1-Heptanol and Cyclohexylmethanol
rhol	859.20	kg/m3	333.15	Density, Viscosity, Refractive Index, and Surface Tension for Six Binary Systems of Adamantane Derivatives with 1-Heptanol and Cyclohexylmethanol
sfust	27.61	J/mol×K	228.20	NIST Webbook
sfust	6.82	J/mol×K	253.60	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C707357&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume