1-Ethyladamantane

Other names: 1-ethyltricyclo[3.3.1.1(3,7)]decane
Inchi: InChI=1S/C12H20/c1-2-12-6-9-3-10(7-12)5-11(4-9)8-12/h9-11H,2-8H2,1H3
InchiKey: LXTHCCWEYOKFSR-UHFFFAOYSA-N
Formula: C12H20
SMILES: CCC12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]: 164.29
CAS: 770-69-4

Physical Properties

Property code	Value	Unit	Source
gf	207.11	kJ/mol	Joback Method
hf	-83.87	kJ/mol	Joback Method
hfus	13.91	kJ/mol	Joback Method
hvap	55.30 ± 1.10	kJ/mol	NIST Webbook
log10ws	-3.56		Crippen Method
logp	3.613		Crippen Method
mcvol	147.360	ml/mol	McGowan Method
pc	2648.83	kPa	Joback Method
rinpol	1234.00		NIST Webbook
rinpol	1240.00		NIST Webbook
rinpol	1249.00		NIST Webbook
rinpol	1259.00		NIST Webbook
rinpol	1234.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1240.00		NIST Webbook
rinpol	1249.00		NIST Webbook
rinpol	1241.90		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1274.00		NIST Webbook
rinpol	1286.00		NIST Webbook
rinpol	1301.00		NIST Webbook
rinpol	1235.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1301.00		NIST Webbook
rinpol	1309.00		NIST Webbook
rinpol	1259.00		NIST Webbook

ripol	1491.00		NIST Webbook
ripol	1469.00		NIST Webbook
ripol	1448.00		NIST Webbook
tb	494.02	K	Joback Method
tc	710.60	K	Joback Method
tf	294.96	K	Joback Method
vc	0.568	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.00	J/mol×K	494.02	Joback Method
cpg	390.28	J/mol×K	530.12	Joback Method
cpg	410.85	J/mol×K	566.21	Joback Method
cpg	429.90	J/mol×K	602.31	Joback Method
cpg	447.62	J/mol×K	638.41	Joback Method
cpg	464.19	J/mol×K	674.50	Joback Method
cpg	479.81	J/mol×K	710.60	Joback Method
hfust	11.28	kJ/mol	190.50	NIST Webbook
hvapt	49.10	kJ/mol	437.50	NIST Webbook
rhol	937.11	kg/m3	293.15	Density, Viscosity, Refractive Index, and Surface Tension for Six Binary Systems of Adamantane Derivatives with 1-Heptanol and Cyclohexylmethanol
rhol	933.58	kg/m3	298.15	Density, Viscosity, Refractive Index, and Surface Tension for Six Binary Systems of Adamantane Derivatives with 1-Heptanol and Cyclohexylmethanol
rhol	929.99	kg/m3	303.15	Density, Viscosity, Refractive Index, and Surface Tension for Six Binary Systems of Adamantane Derivatives with 1-Heptanol and Cyclohexylmethanol

rhol	926.40	kg/m3	308.15	Density, Viscosity, Refractive Index, and Surface Tension for Six Binary Systems of Adamantane Derivatives with 1-Heptanol and Cyclohexylmethanol
rhol	922.81	kg/m3	313.15	Density, Viscosity, Refractive Index, and Surface Tension for Six Binary Systems of Adamantane Derivatives with 1-Heptanol and Cyclohexylmethanol
rhol	919.21	kg/m3	318.15	Density, Viscosity, Refractive Index, and Surface Tension for Six Binary Systems of Adamantane Derivatives with 1-Heptanol and Cyclohexylmethanol
rhol	915.62	kg/m3	323.15	Density, Viscosity, Refractive Index, and Surface Tension for Six Binary Systems of Adamantane Derivatives with 1-Heptanol and Cyclohexylmethanol
rhol	912.01	kg/m3	328.15	Density, Viscosity, Refractive Index, and Surface Tension for Six Binary Systems of Adamantane Derivatives with 1-Heptanol and Cyclohexylmethanol
rhol	908.41	kg/m3	333.15	Density, Viscosity, Refractive Index, and Surface Tension for Six Binary Systems of Adamantane Derivatives with 1-Heptanol and Cyclohexylmethanol

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45208e+01
Coeff. B	-4.57869e+03
Coeff. C	-3.75610e+01
Temperature range (K), min.	359.25
Temperature range (K), max.	534.74

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C770694&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
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
rhol:	Liquid 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