Adamantane, 1-chloro-

Other names:	1-chloroadamantane
	1-chlorotricyclo[3.3.1.1(3,7)]decane
	Tricyclo[3.3.1.1
	tricyclo[3.3.1.1(3,7)]decane, 1-chloro-
Inchi:	InChI=1S/C10H15Cl/c11-10-4-7-1-8(5-10)3-9(2-7)6-10/h7-9H,1-6H2
InchiKey:	OZNXTQSXSHODFR-UHFFFAOYSA-N
Formula:	C10H15Cl
SMILES:	ClC12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]:	170.68
CAS:	935-56-8

Physical Properties

Property code	Value	Unit	Source
gf	178.34	kJ/mol	Joback Method
hf	-58.33	kJ/mol	Joback Method
hfus	5.96	kJ/mol	Relationship between the two-component system 1-Br-adamantane + 1-Cl-adamantane and the high-pressure properties of the pure components
hvap	40.69	kJ/mol	Joback Method
ie	9.30	eV	NIST Webbook
log10ws	-3.23		Crippen Method
logp	3.194		Crippen Method
mcvol	131.420	ml/mol	McGowan Method
pc	3127.99	kPa	Joback Method
rinpol	1286.00		NIST Webbook
rinpol	1300.00		NIST Webbook
rinpol	1315.00		NIST Webbook
rinpol	1316.00		NIST Webbook
rinpol	1316.00		NIST Webbook
rinpol	1300.00		NIST Webbook
rinpol	1350.00		NIST Webbook
rinpol	1300.00		NIST Webbook
rinpol	1298.00		NIST Webbook
rinpol	1298.00		NIST Webbook
rinpol	1331.00		NIST Webbook
rinpol	1341.00		NIST Webbook

rinpol	1300.00		NIST Webbook
rinpol	1300.00		NIST Webbook
rinpol	1298.00		NIST Webbook
rinpol	1298.00		NIST Webbook
rinpol	1315.00		NIST Webbook
ripol	1691.00		NIST Webbook
ripol	1691.00		NIST Webbook
ripol	1741.00		NIST Webbook
ripol	1713.00		NIST Webbook
ripol	1689.00		NIST Webbook
ripol	1691.00		NIST Webbook
tb	485.69	K	Joback Method
tc	715.28	K	Joback Method
tf	442.50 ± 0.20	K	NIST Webbook
vc	0.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	391.90	J/mol×K	677.02	Joback Method
cpg	405.25	J/mol×K	715.28	Joback Method
cpg	307.47	J/mol×K	485.69	Joback Method
cpg	327.45	J/mol×K	523.96	Joback Method
cpg	345.66	J/mol×K	562.22	Joback Method
cpg	362.33	J/mol×K	600.49	Joback Method
cpg	377.67	J/mol×K	638.75	Joback Method
hfust	4.87	kJ/mol	442.50	NIST Webbook
hfust	6.01	kJ/mol	244.20	NIST Webbook
hfust	5.53	kJ/mol	439.70	NIST Webbook
hfust	4.87	kJ/mol	442.50	NIST Webbook
sfust	11.01	J/mol×K	442.50	NIST Webbook
sfust	24.61	J/mol×K	244.20	NIST Webbook

Sources

Relationship between the two-component system 1-Br-adamantane + 1-Cl-adamantane and the high-pressure properties of the pure components:	https://www.doi.org/10.1016/j.fluid.2017.07.020
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=C935568&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
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