

1-Ethyl-3-vinyl-adamantane

Inchi:	InChI=1S/C14H22/c1-3-13-6-11-5-12(7-13)9-14(4-2,8-11)10-13/h3,11-12H,1,4-10H2,2H3
InchiKey:	AVRIJUMTHPONKV-UHFFFAOYSA-N
Formula:	C14H22
SMILES:	<chem>C=CC12CC3CC(C1)CC(CC)(C3)C2</chem>
Mol. weight [g/mol]:	190.32

Physical Properties

Property code	Value	Unit	Source
gf	306.30	kJ/mol	Joback Method
hf	15.52	kJ/mol	Joback Method
hfus	11.52	kJ/mol	Joback Method
hvap	43.39	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	4.169		Crippen Method
mcvol	171.240	ml/mol	McGowan Method
pc	2384.19	kPa	Joback Method
rinpol	1514.00		NIST Webbook
rinpol	1514.00		NIST Webbook
tb	536.70	K	Joback Method
tc	759.93	K	Joback Method
tf	339.64	K	Joback Method
vc	0.658	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.34	J/mol×K	536.70	Joback Method
cpg	470.63	J/mol×K	573.90	Joback Method
cpg	491.13	J/mol×K	611.11	Joback Method
cpg	510.14	J/mol×K	648.31	Joback Method
cpg	527.99	J/mol×K	685.52	Joback Method
cpg	544.97	J/mol×K	722.72	Joback Method
cpg	561.41	J/mol×K	759.93	Joback Method

Sources

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=U214996&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.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
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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