2-(2-adamantyl)propene

Inchi: InChI=1S/C13H20/c1-8(2)13-11-4-9-3-10(6-11)7-12(13)5-9/h9-13H,1,3-7H2,2H3
InchiKey: VLJRVQFLGRFPSF-UHFFFAOYSA-N
Formula: C13H20
SMILES: C=C(C)C1C2CC3CC(C2)CC1C3
Mol. weight [g/mol]: 176.30

Physical Properties

Property code	Value	Unit	Source
gf	292.60	kJ/mol	Joback Method
hf	-24.45	kJ/mol	Joback Method
hfus	21.28	kJ/mol	Joback Method
hvap	43.23	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	3.635		Crippen Method
mcvol	157.150	ml/mol	McGowan Method
pc	2333.78	kPa	Joback Method
rinpol	1422.00		NIST Webbook
rinpol	1409.00		NIST Webbook
rinpol	1394.00		NIST Webbook
rinpol	1382.00		NIST Webbook
ripol	1691.00		NIST Webbook
ripol	1667.00		NIST Webbook
ripol	1643.00		NIST Webbook
tb	508.55	K	Joback Method
tc	721.37	K	Joback Method
tf	262.37	K	Joback Method
vc	0.607	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.36	J/mol×K	508.55	Joback Method
cpg	421.21	J/mol×K	544.02	Joback Method
cpg	442.55	J/mol×K	579.49	Joback Method

cpg	462.48	J/mol×K	614.96	Joback Method
cpg	481.09	J/mol×K	650.43	Joback Method
cpg	498.49	J/mol×K	685.90	Joback Method
cpg	514.78	J/mol×K	721.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R304511&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
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
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